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Supporting Information

Synthesis and conformational preferences of peptides and proteins with cysteine sulfonic acid

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Materials

Amino acids and resins for peptide synthesis were purchased from Chem-Impex. Hexafluorophosphate benzotriazole-N,N,N',N'-tetramethyl-uronium (HBTU), diisopropylethylamine (DIPEA), and trifluoroacetic acid (TFA) were purchased from Chem-Impex. Methyltrioxorhenium (MTO) was purchased from Strem Chemicals. Triisopropylsilane (TIS) was purchased from Acros Organics. N, N-Dimethylformamide (DMF), acetonitrile (CH_3CN), and other compounds were purchased from Fisher Scientific unless otherwise indicated. Peptides were synthesized using a Protein Technologies Inc. Tribute or a PS3 peptide synthesizer. The modifications to the synthesized peptides were performed manually on the solid phase or in solution phase. In all reactions and solutions, ultrapure water purified by a Millipore Synergy 185 water purification system with a Simpak-2 cartridge was used. Peptide concentrations were determined by UV/Vis absorbance based on tyrosine absorbance (ε = 1280 M^{-1} cm^{-1} at 280 nm in water) on a Thermo Scientific NanoDrop spectrophotometer. All compounds were used as purchased, with no additional purification performed.

Peptide synthesis and characterization

Peptides (0.1 or 0.25 mmol) were synthesized on Rink amide resin via standard Fmoc solid-phase peptide synthesis using HBTU as a coupling reagent on a Tribute peptide synthesizer or a Rainin PS3 peptide synthesizer. The resin was allowed to swell in DMF (2 × 15 minutes) before the start of peptide synthesis. Standard amino acid couplings were accomplished via reaction for 1 hour at room temperature using 4 equivalents of HBTU and 4 equivalents of Fmoc amino acid. Each cycle of amide coupling involved the following four steps: (1) removal of the Fmoc protecting group in 20% piperidine in DMF, 3 × 5 minutes; (2) resin wash in DMF, 5 × 1 minute; (3) amino acid coupling (Fmoc amino acid, HBTU, and 8% DIPEA in DMF; 1 hour or 4 hours); (4) resin wash with DMF, 3 × 1 minute. After the addition of the final residue, the N-terminus of the peptide was deprotected (20% piperidine in DMF, 3 × 5 minutes) and subsequently acetylated using 10% acetic anhydride in pyridine (3 × 5 minutes). Finally, the resin was washed with DMF (6 × 1 minute, CH_2Cl_2 (3 × 1 minute), and diethyl ether (1 × 1 minute). Cleavage of peptides from resin and deprotection of side chains other than cysteine was accomplished using 95% TFA/5% TIS, with stirring, for 1–3 hours. All peptides contained C-terminal amides after cleavage from the resin. TFA was removed under nitrogen via evaporation, and peptides were precipitated in ice-cold diethyl ether. The precipitated peptides were dried in air and dissolved in water and filtered. Peptides were purified to homogeneity by reverse phase analytical HPLC (Varian Microsorb MV analytical C18, 4.6 × 250 mm, 5 μm particle size, 100 Å pore). Peptides were purified to homogeneity using a linear gradient of buffer B (20% water, 80% CH_3CN, 0.05% TFA) in buffer A (98% H_2O, 2% CH_3CN, 0.06% TFA) over 60 minutes and lyophilized overnight in a Labonco CentriVap Concentrator. The purity of peptides was verified by reinjection on analytical HPLC. Peptides were characterized by ESI-MS (positive ion mode or negative ion mode) on a Waters ACQUITY UPLC H-Class/SQD2 mass spectrometer. Expected and observed peptide masses are indicated as $[M+H]^+$, $[M/2+H]^+$, or $[M+Na]^+$. Analytical data for peptides are in Table S1. The concentrations of peptides containing tyrosine residue were determined by UV-Vis spectroscopy based on tyrosine absorbance (ε_{280} = 1280 M^{-1} cm^{-1} in water).

Solution-phase synthesis of peptides containing cysteine sulfonic acid

Cysteine was incorporated on the peptide at the respective position via solid-phase peptide synthesis using triphenylmethyl-protected (trityl-protected) cysteine to obtain Ac-GPP-C(Trt)-PPGY-NH_2 peptide on Rink amide resin. The cleavage and deprotection of the resin-bound peptide was performed using 95% TFA/5% triisopropylsilane, with stirring for 2 hours. Purified peptide (Ac-GPP-C(SH)-PPGY-NH_2) was obtained using a gradient of 0-25% buffer B in buffer A over 60 minutes using a C18 analytical column. The obtained pure peptide was lyophilized overnight in a Labonco CentriVap Concentrator. To a solution of H_2O_2 (30% in water, 50 μL) was added a solution of methyltrioxorhenium (MTO, 100 μL, 1.5 mg/mL in CH_3CN). The mixture was vortexed and incubated at ambient temperature for 1 minute. The purified and lyophilized peptide in a 1.5 mL Eppendorf tube was dissolved in 50 μL of water, and 300 μL of CH_3CN were added to make the final volume 350 μL. The MTO mixture made in the previous step was then added to the peptide solution. The reaction was incubated at ambient temperature for 30 minutes to produce the oxidized peptide Ac-GPP-C(SO_3^-)-PPGY-NH_2. Then, 2.5 mL of water was added to the reaction mixture to make the final volume of 3 mL. The excess of H_2O_2 was quenched with approximately 10 mg of dithiothreitol (DTT), vortexed, and incubated at room temperature for 10 minutes. Then the reaction mixture was filtered and purified via analytical HPLC using a gradient of 0-25% buffer B in buffer A over 60 minutes.

Solid-phase synthesis of peptides containing cysteine sulfonic acid

Peptides (Ac-C(Trt)-PPG-Y(*t*Bu)-NH-resin and Ac-A-C(Trt)-AAAA-K(Boc)-AAAA-K(Boc)-AAG-Y(*t*Bu)-NH-resin) containing trityl-protected cysteine were synthesized via standard solid-phase peptide synthesis method on Rink amide resin. The N-terminus of the peptides were acylated after removing the Fmoc protecting group. The trityl group was selectively removed by 1% TFA/5% TIS in CH_2Cl_2 for 5 minutes. The process was repeated until the yellow color disappeared. The resin was then washed with CH_2Cl_2 (3 × 1 minute) and DMF (3 × 1 minute). To a solution of H_2O_2 (30% in water, 100 μL) was added a solution of Methyltrioxorhenium (MTO, 200 μL, 1.5 mg/mL in CH_3CN). The mixture was vortexed for 1 minute and incubated at ambient temperature for another 1 minute. The 3 mL of CH_2Cl_2:CH_3CN in the ratio of 1:1 was added to the MTO mixture, added to the resin in fritted column, and allowed to react for 2 hours at room temperature in a rotating shaker. The resin was washed with DMF (3 × 1 minute), CH_2Cl_2 (3 × 1 minute), and dried with diethyl ether. Cleavage of peptides from resin and deprotection of side chains was accomplished using 95% TFA/5% TIS, with stirring, for 1–3 hours. The peptide was subjected to ether precipitation in the ice bath for 10 minutes and centrifuged at 13000 rpm for 2 minutes. Then the precipitated peptide was air-dried, dissolved in water, and filtered. The obtained peptide Ac-C(SO_3^-)-PPGY-NH_2 was purified via analytical HPLC using a gradient of 0-20% buffer B in buffer A over 60 minutes, and peptide Ac-AC(SO_3^-)-AAAAKAAAAKAAGY-NH_2 was purified via analytical HPLC using a gradient of 0-35% buffer B in buffer A over 60 minutes. Both peptides with cysteine sulfonic acid were analyzed and confirmed via ESI mass spectrometry and NMR spectroscopy.

Solid-phase oxidation of peptide to synthesize peptides containing cysteine sulfinic acid

Cysteine was incorporated on the solid phase by coupling *N*-Fmoc-S-4-methoxybenzylsulfonyl cysteine (Fmoc-Cys(Mob)-OH) to the growing peptide at its respective position to obtain peptides Ac-C(Mob)-PPG-Y(*t*Bu)-NH-resin and Ac-A-C(Mob)-AAAA-K(Boc)-AAAA-K(Boc)-AAG-Y(*t*Bu)-NH-resin on Rink amide resin. The N-termini of the peptides were acylated after removing the Fmoc group. The resin was then washed with CH_2Cl_2 (3 × 1 minute) and DMF (3 × 1 minute). To a solution of H_2O_2 (30% in water, 100 μL) was added a solution of methyltrioxorhenium (MTO, 200 μL, 1.5 mg/mL in CH_3CN). The mixture was vortexed and incubated at ambient temperature for 1 minute. Afterwards, a solution of CH_2Cl_2:CH_3CN (1:1) was added to the mixture to bring the final volume 3 mL. This final mixture, containing H_2O_2, MTO, CH_2Cl_2, and CH_3CN, was then added to the resin in the fritted column and allowed to react for 2 hours at room temperature. The resin was washed with DMF (3 × 1 minute), CH_2Cl_2 (3 × 1 minute), and dried with diethyl ether. Cleavage of peptides from resin and removal of protecting groups other than Mob was accomplished using 95% TFA/5% TIS, with stirring, for 1 hour to obtain the peptides Ac-C(SO_2Mob)-PPGY-NH_2 and Ac-A-C(SO_2Mob)-AAAAKAAAAKAAGY-NH_2. Peptides were subjected to ether precipitation in the ice bath for 10 minutes and centrifuged at 13000 rpm for 2 minutes. Then the precipitated peptides were air-dried, dissolved in water, and filtered. The obtained peptide, Ac-C(SO_2Mob)-PPGY-NH_2, was purified via analytical HPLC using a gradient of 0-25% buffer B in buffer A over 60 minutes, and Ac-A-C(SO_2Mob)-AAAAKAAAAKAAGY-NH_2 peptide was purified via analytical HPLC using a gradient of 0-40% buffer B in buffer A over 60 minutes. The purified peptides were then lyophilized overnight in a Labonco CentriVap Concentrator. A solution of 50% triflic acid (TfOH), 45% TFA, and 5% H_2O was prepared, chilled on ice, and used for the deprotection of the Mob group. Approximately 300 μL of this mixture was added to the purified and lyophilized peptide, and the resulting solution was stirred at room temperature. A faint pink color developed quickly, deepening to purple over the reaction. After 10-20 minutes of the reaction, the solution was chilled on ice, and chilled water was added dropwise, bringing the solution volume to approximately 3 mL. The reaction mixture was partially neutralized by gradually adding solid $NaHCO_3$ (about 0.5 g) to a pH (~2) of HPLC buffer. The resulting solutions containing peptides were filtered and subjected to HPLC purification. The peptide Ac-C(SO_2^-)-PPGY-NH_2 was purified via analytical HPLC using a gradient of 0-20% buffer B in buffer A over 60 minutes, and the peptide Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2 was purified via analytical HPLC using a gradient of 0-40% buffer B in buffer A over 60 minutes.

Danger! Triflic acid (TfOH) is a very strong acid (p*K*a –14) that can cause severe burns on contact with the skin, and inhalation can lead to fatal spasms, inflammation, and edema. To prevent exposure to fumes, accidental inhalation, and skin or eye contact, TfOH must be added dropwise to ice-cold TFA/H_2O in a fume hood. TfOH is transferred with a glass Pasteur pipette, using all personal safety protection, and using the sash of the fume hood as a glass safety barrier to prevent exposure due to potential splashing during transfer.

Characterization data for peptides

peptide	t_R, min	calculated mass, $[M+H]^+$	observed mass
Ac-GPP-C(SH)-PPGY-NH_2	52.5[a]	828.4	828.9
Ac-GPP-C(SO_3^-)-PPGY-NH_2	39.5[a]	876.4	876.5
Ac-C(SH)-PPGY-NH_2	40.5[b]	577.2	577.3
Ac-C(SO_2Mob)-PPGY-NH_2	48.5[a]	729.3	751.3[e]
Ac-C(SO_2^-)-PPGY-NH_2	22.5[b]	609.2	609.2
Ac-C(SO_3^-)-PPGY-NH_2	23.5[b]	625.2	623.7[f]
Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2	55.5[c]	1420.7	1420.7
Ac-A-C(SO_2Mob)-AAAAKAAAAKAAGY-NH_2	58.5[d]	1572.8	1573.0
Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2	47.5[d]	1452.7	727.2[g]
Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2	46.5[c]	1468.7	1469.5

Table S1. Characterization data for peptides.
Retention times (t_R) of peptides, with calculated and observed masses ($[M+H]^+$ by ESI-MS in positive ion mode) indicated. Unless noted otherwise, all peptides contained C-terminal amides and were purified using an analytical HPLC column.
[a] Peptide was purified using a linear gradient of 0-25% buffer B in buffer A over 60 minutes.
[b] Peptide was purified using a linear gradient of 0-20% buffer B in buffer A over 60 minutes.
[c] Peptide was purified using a linear gradient of 0-35% buffer B in buffer A over 60 minutes.
[d] Peptide was purified using a linear gradient of 0-40% buffer B in buffer A over 60 minutes.
[e] Peptide was detected at $[M+Na]^+$.
[f] Peptide was detected at $[M–H]^–$

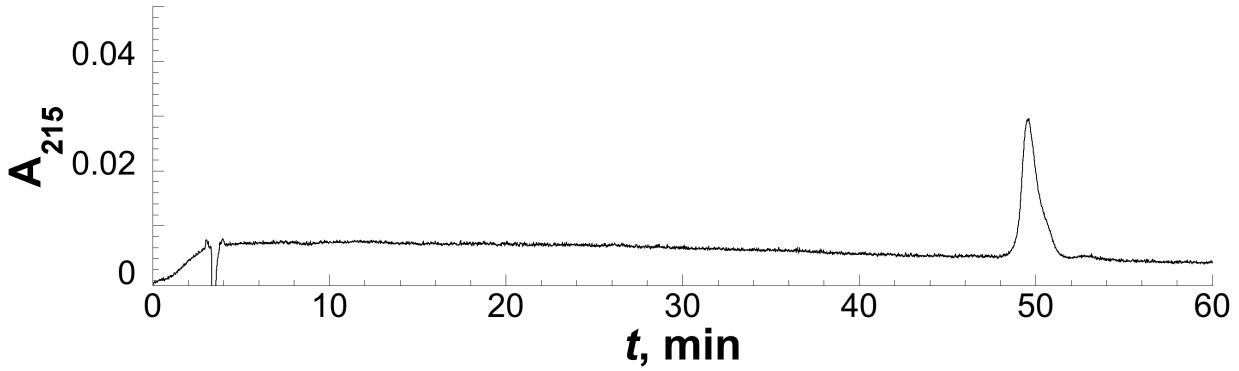


Figure S1. HPLC chromatogram of purified Ac-GPP-C(SH)-PPGY-NH_2. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-25% buffer B in buffer A over 60 minutes.

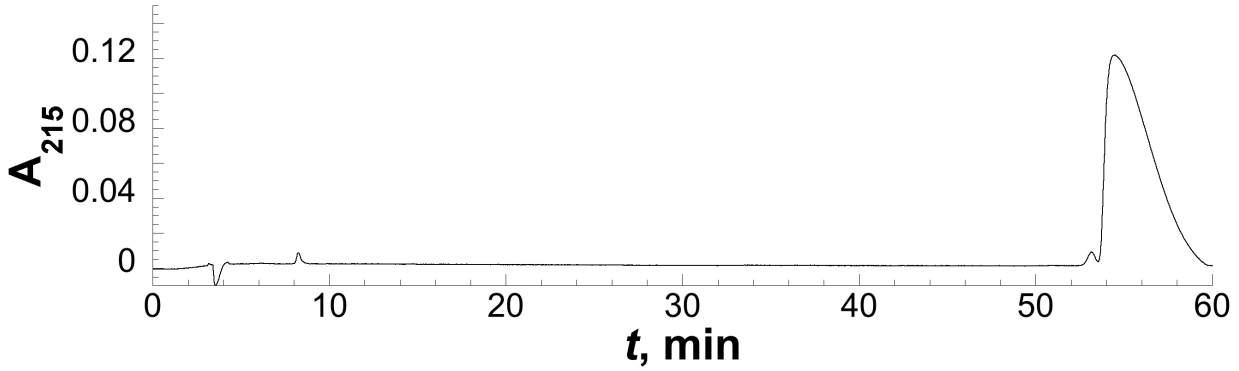


Figure S2. HPLC chromatogram of purified Ac-C(SO_2-Mob)-PPGY-NH_2. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-25% buffer B in buffer A over 60 minutes.

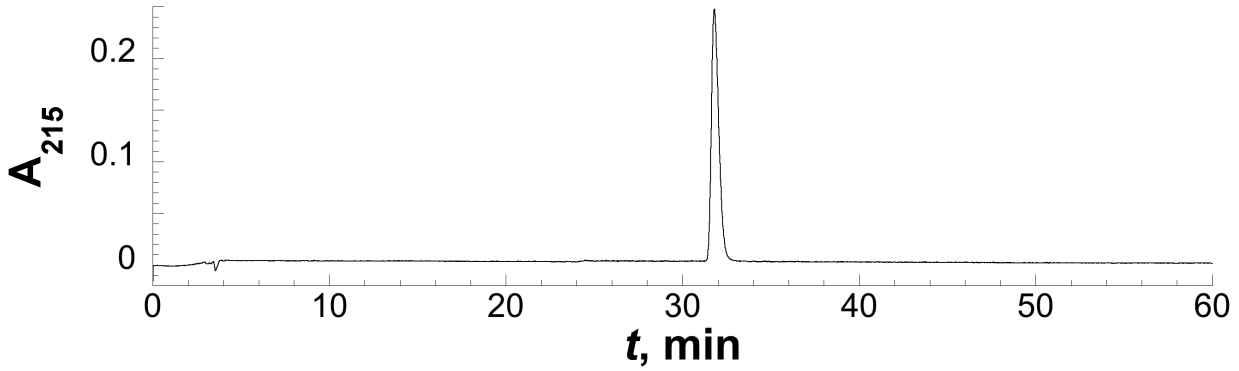


Figure S3. HPLC chromatogram of purified Ac-C(SO_2^-)-PPGY-NH_2. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-20% buffer B in buffer A over 60 minutes.

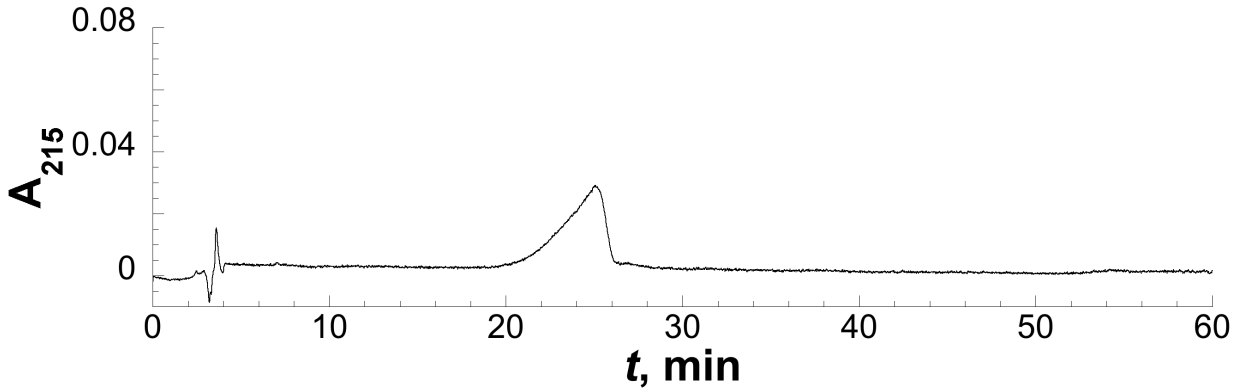


Figure S4. HPLC chromatogram of purified Ac-C(SO_3^-)-PPGY-NH_2. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-15% buffer B in buffer A over 60 minutes.

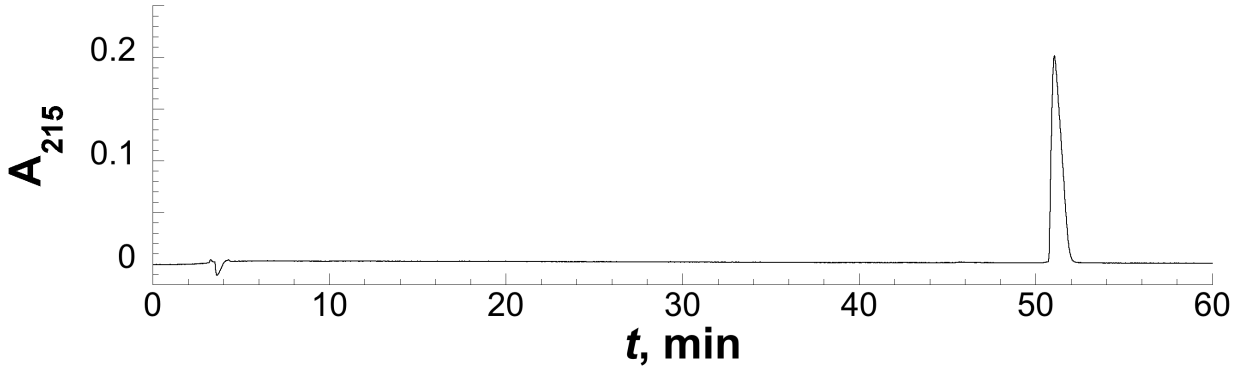


Figure S5. HPLC chromatogram of purified Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-30% buffer B in buffer A over 60 minutes.

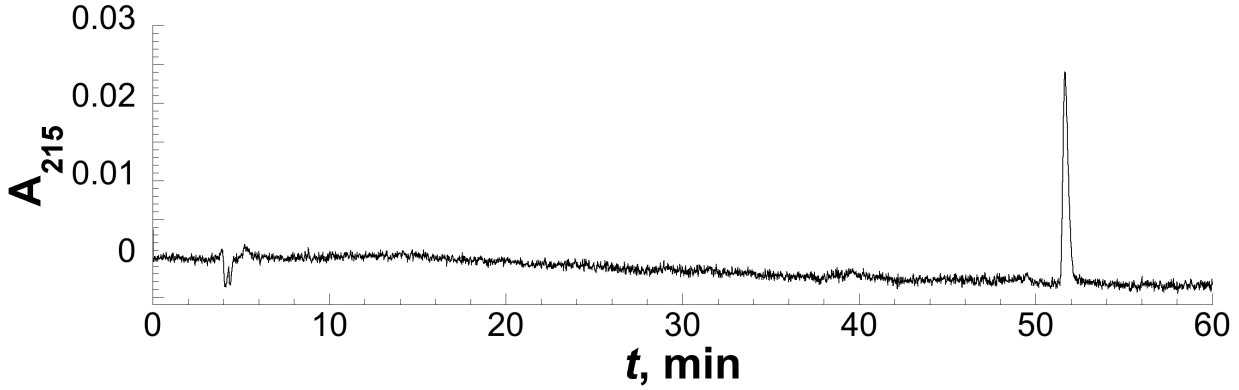


Figure S6. HPLC chromatogram of purified Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-35% buffer B in buffer A over 60 minutes.

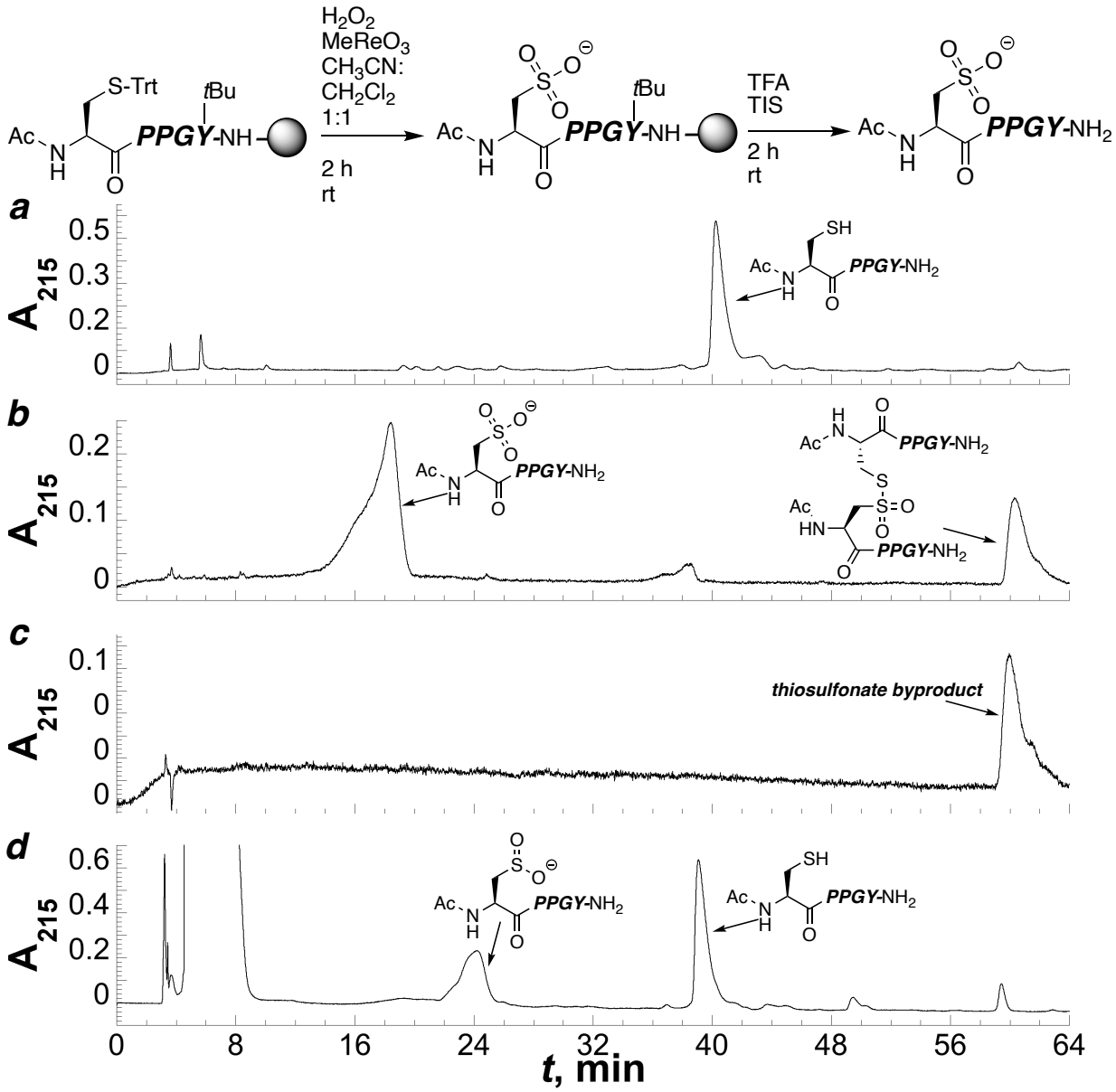
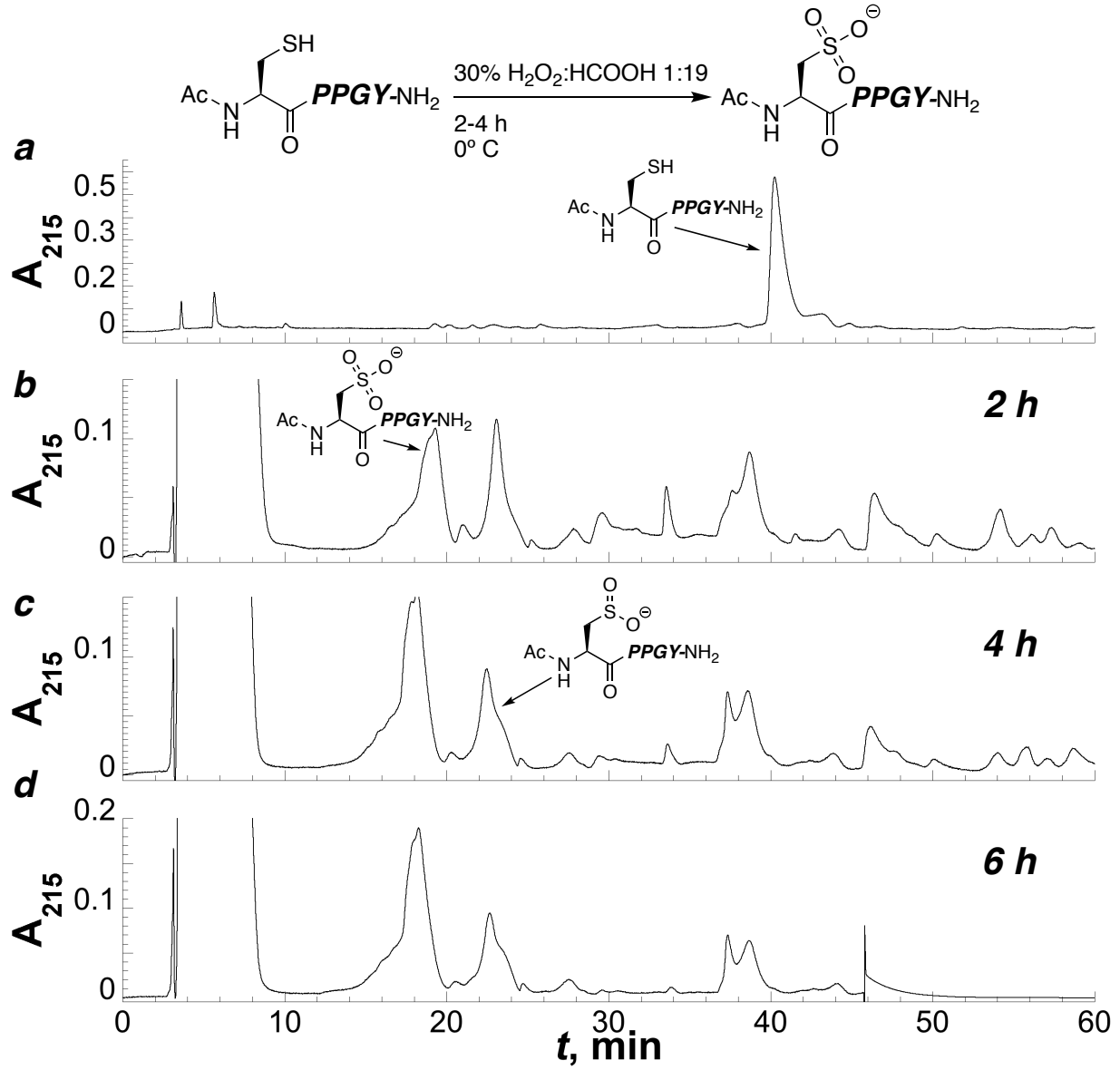


Figure S7. Solid-state oxidation of the peptide using $MeReO_3/H_2O_2$ without trityl group deprotection. (a) HPLC chromatogram of the peptide (Ac-C(SH)-PPGY-NH_2) prior to oxidation, after cleavage from resin, and deprotection. (b) Crude HPLC chromatogram of the peptide on resin after oxidation with 0.3 M H_2O_2 catalyzed by 0.4 mM $MeReO_3$ in CH_3CN:CH_2Cl_2 1:1 for 2 hours at room temperature, followed by cleavage from resin and deprotection with TFA/TIS 95%/5% for 2 hours at room temperature. (c) HPLC chromatogram of the thiosulfonate byproduct of the peptide. (d) HPLC chromatogram of the thiosulfonate byproduct of the peptide after reaction with approximately 10 mg of DTT added to the solution. Analytical HPLC was conducted on a C18 column using a linear gradient of 0-20% buffer B in buffer A over 60 minutes.

Figure S8. HPLC chromatograms of the synthesis of Ac-C(SO_3^-)-PPGY-NH_2 using performic



acid. (a) HPLC chromatogram of starting peptide Ac-C(SH)-PPGY-NH_2 before oxidation with performic acid. The HPLC purified and freeze-dried peptide was subjected to oxidation with 250 µL of performic acid (30% H_2O_2:formic acid 1:19) in ice. A 25 µL samples were withdrawn from the reaction mixture at (b) 2 hours, (c) 4 hours, and (d) 6 hours and diluted with 500 µL water before storing at –20 ºC. Excess performic acid in these samples was quenched with 50 µL of 1 M DTT before performing analytical HPLC on a C18 column using a linear gradient of 0-20% buffer B in buffer A over 60 minutes. The product peak was found to increase as time increased. However, the reaction side products also increased with time.

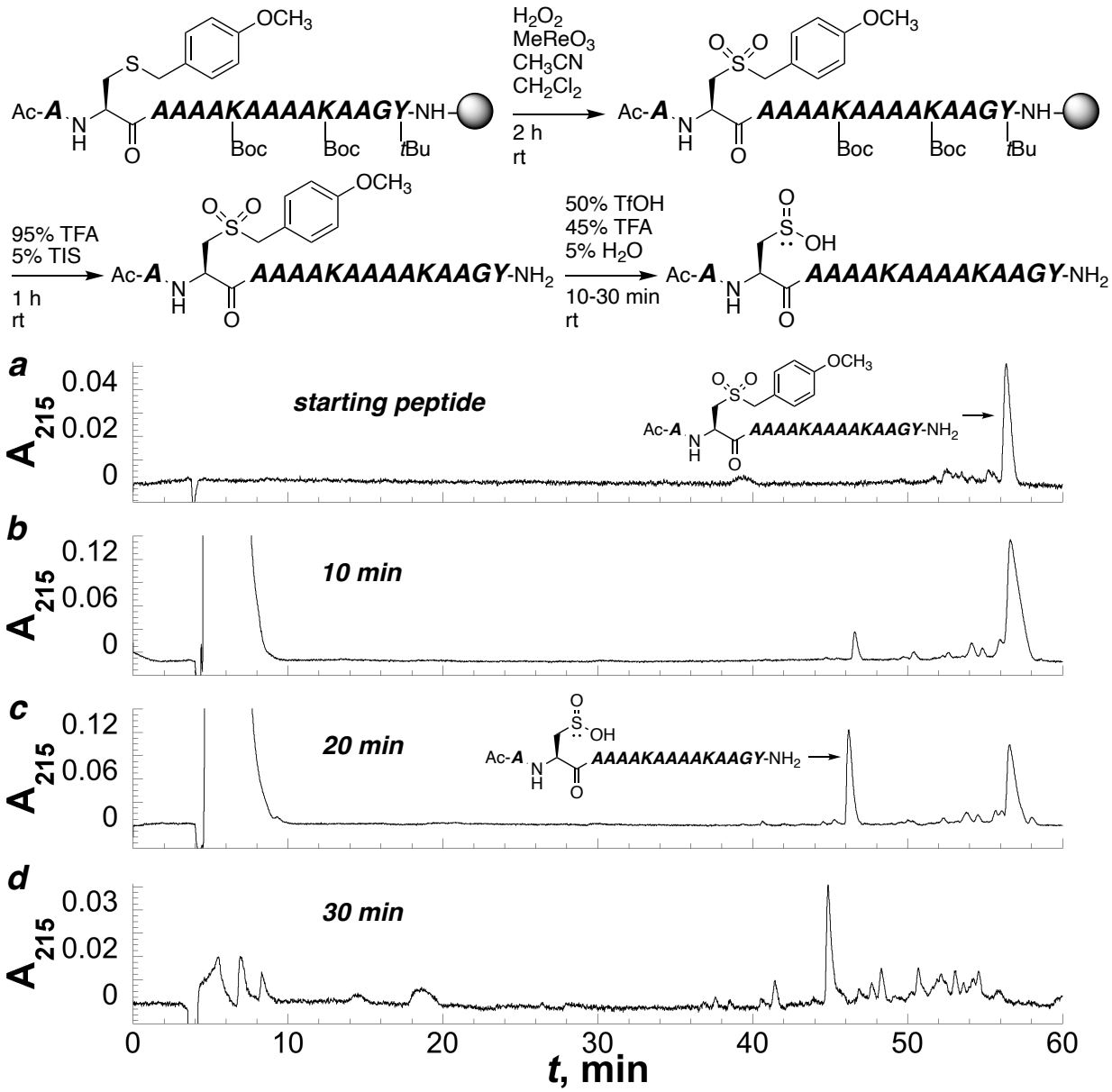


Figure S9. Oxidation of Mob-protected cysteine in a peptide with $MeReO_3/H_2O_2$ on solid phase to generate the peptide with cysteine sulfinic acid**.** (a) HPLC chromatogram of the starting peptide Ac-A-C(SO_2Mob)-AAAAKAAAAKAAGY-NH_2 synthesized via solid-phase oxidation with 0.3 M H_2O_2 catalyzed by 0.4 mM $MeReO_3$ in CH_3CN:CH_2Cl_2 1:1 for 2 hours at room temperature, followed by cleavage from resin and deprotection of protecting group other than Mob with 95% TFA/5% TIS for 2 hours at room temperature. Crude HPLC chromatogram of the purified peptide from (a) after 4-methoxybenzyl (Mob) deprotection with 50% TfOH/45% TFA/5% H_2O for (b) 10 minutes, (c) 20 minutes, and (d) 30 minutes at room temperature. HPLC analysis was conducted using an analytical C18 column with a linear gradient of 0% to 40% buffer B in buffer A over 60 minutes.

Circular dichroism (CD) spectroscopy

Circular dichroism (CD) experiments were conducted on a Jasco model J-810 or J-1500 spectropolarimeter. All data were collected using a 1 mm cell (Starna Cells, Atascadero, CA). CD spectra were collected at 0.5˚ C or 25 ˚C with 50-150 μM peptide in 5 mM phosphate buffer (pH 4.0 or pH 7.0 or 8.5) containing 25 mM KF. Data are the average of at least three independent trials. Individual spectra were collected every nm with an averaging time of 8 s and at least three accumulations. The data represent the average of at least three independent trials. The concentrations of peptides were determined by UV-Vis spectroscopy based on tyrosine absorbance (ε_{280} = 1280 M^{-1} cm^{-1} in water). Error bars are shown and indicate standard error. Data were background corrected but not smoothed.

Ac-GPP**X**PPGY-NH_2 **X=**	λ_{max}, nm	$[\theta]_{228}$, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$	[θ] at λ_{max}, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$
Pro	230	3000	± 170	3070	± 250
Cys-SH	232	–680	± 60	–240	± 90
Cys-S^-	233	–530	± 80	–260	± 60
Cys-SO_2^-	231	340	± 120	1290	± 180
Cys-SO_3^-	230	310	± 70	340	± 50

Table S2. Summary of circular dichroism data with standard error for polyproline helix propagation model peptide Ac-GPPXPPGY-NH_2.

Ac-**X**PPGY-NH_2 **X=**	λ_{max}, nm	$[\theta]_{228}$, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$	[θ] at λ_{max}, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$
Ala	227	3180	± 40	3260	± 50
Cys-SH	230	1120	± 60	1190	± 70
Cys-S^-	226	2400	± 50	2540	± 60
Cys-SO_2^-	232	2690	± 60	2980	± 40
Cys-SO_3^-	227	2340	± 130	2380	± 120

Table S3. Summary of circular dichroism data with standard error for the polyproline helix initiation model peptide Ac-XPPGY-NH_2.

Ac-A**X**AAA AKAAAAK AAGY-NH_2 **X=**	$[\theta]_{208}$, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$	$[\theta]_{222}$, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$	$[\theta]_{190}$, deg cm^2 $dmol^{-1}$	error, deg cm^2 $dmol^{-1}$
Lys	–18800	±170	–17800	±40	31500	±880
Cys-SH	–18600	±670	–17300	±670	28400	±1220
Cys-S^-	–20600	±280	–20200	±320	38000	±860
Cys-SO_2^-	–24100	±230	–24200	±240	51600	±456
Cys-SO_3^-	–21200	±650	–20800	±690	38900	±1540

Table S4. Summary of circular dichroism data with standard error for α-helical peptides.

NMR spectroscopy of peptides

NMR spectra of peptides were acquired at 300 K or 274 K on a Brüker AVC 400 MHz NMR spectrometer equipped with a triple resonance cryoprobe or a TXI probe. Each peptide was dissolved in a solution containing 5 mM phosphate buffer (pH 4.0) and 25 mM NaCl in 90% H_2O/10% D_2O. The pH of each sample was recorded and adjusted as necessary using dilute HCl or NaOH. All NMR spectra were internally referenced with 100 μM trimethylsilylpropanoic acid (TSP). NMR spectra (1-D) were collected with an excitation sculpting pulse sequence and a relaxation delay of 2 s. Coupling constants between the amide and α-protons ($^3J_{\alpha N}$) were determined directly from the 1-D spectra. TOCSY NMR spectra were collected with an excitation sculpting TOCSY pulse sequence, sweep widths of 12.25 ppm in t_1 and t_2, 512 × 1024 complex data points, 8 scans per t_1 increment, a relaxation delay of 1.7 s, an acquisition time of 0.213 s, and a TOCSY mixing time of 80 ms. All resonances were calibrated with respect to TSP, which was set to 0.00 ppm. The 1-D NMR data were processed in MestReNova, version 11.0.4, and TOCSY NMR spectra were processed in Sparky.

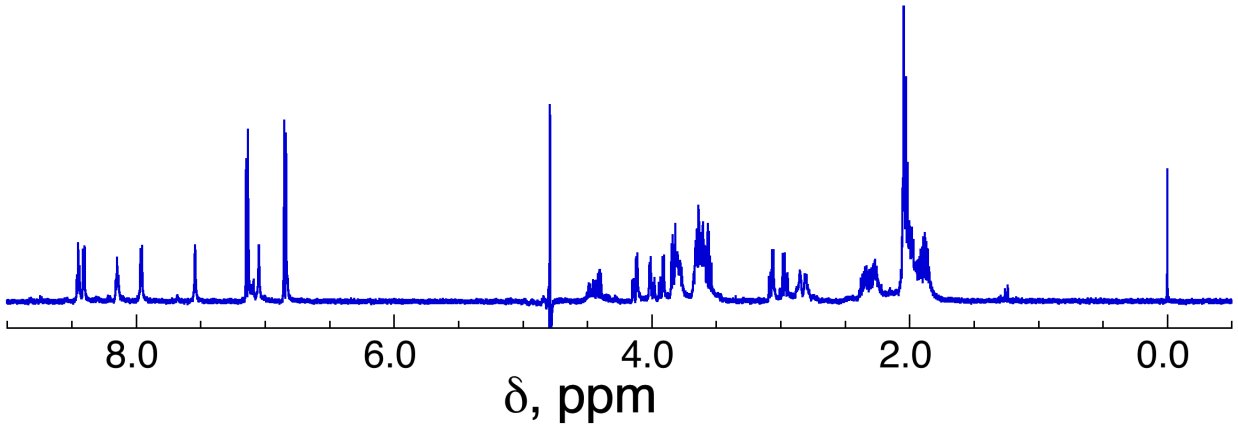


Figure S10. ^{1}H NMR spectrum of the peptide Ac-GPP-C(SH)-PPGY-NH_2 at 300 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

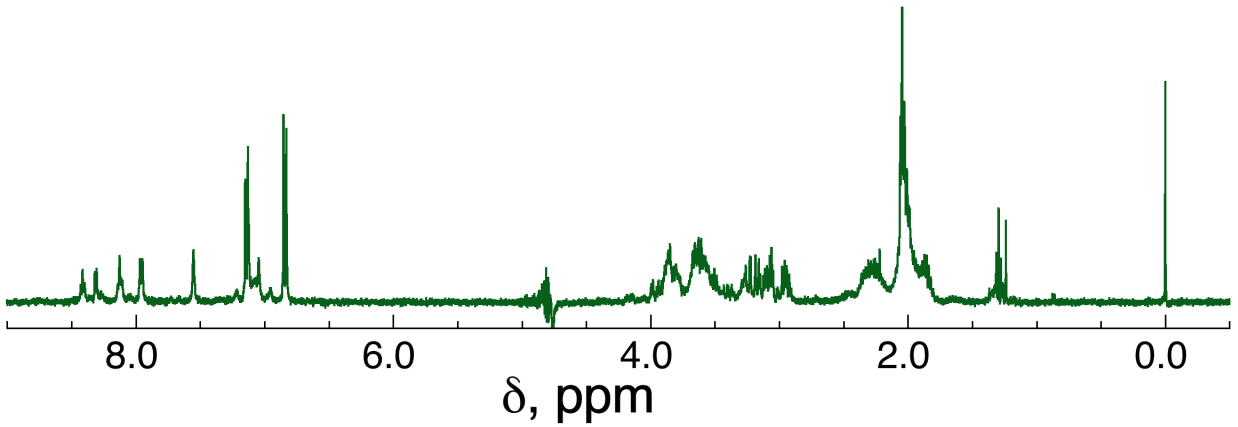


Figure S11. ^{1}H NMR spectrum of the peptide Ac-GPP-C(SO_3^-)-PPGY-NH_2 at 300 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

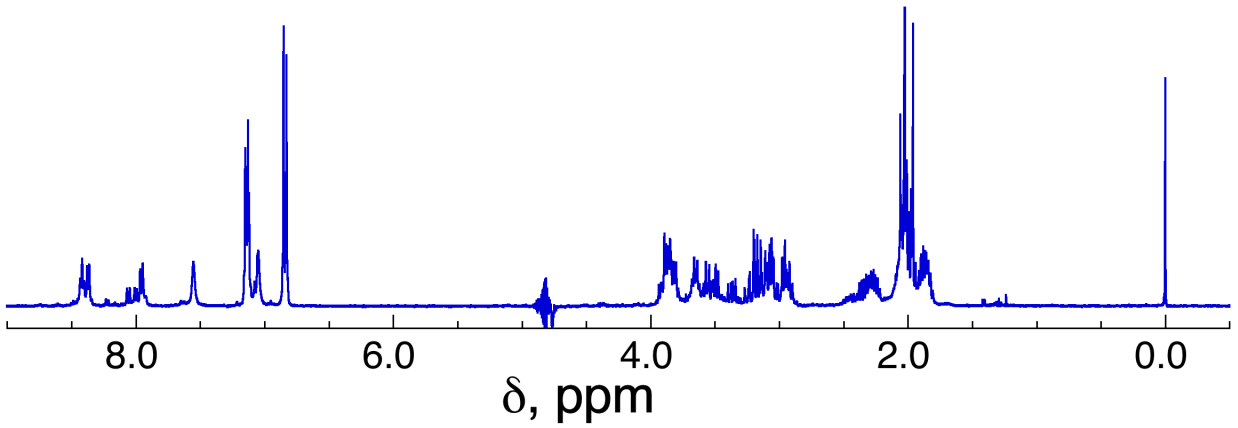


Figure S12. ^{1}H NMR spectrum of the peptide Ac-C(SH)-PPGY-NH_2 at 300 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

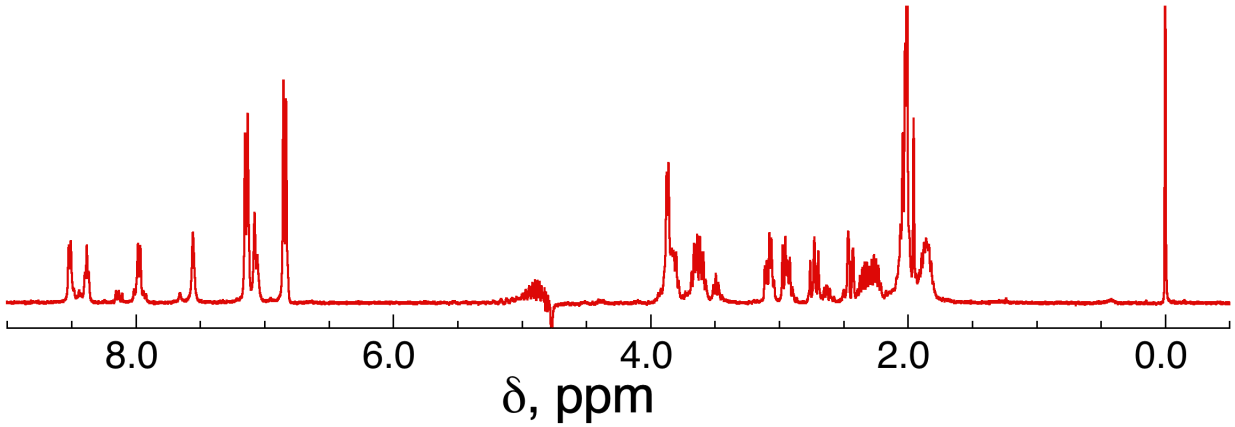


Figure S13. ^{1}H NMR spectrum of the peptide Ac-C(SO_2^-)-PPGY-NH_2 at 300 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

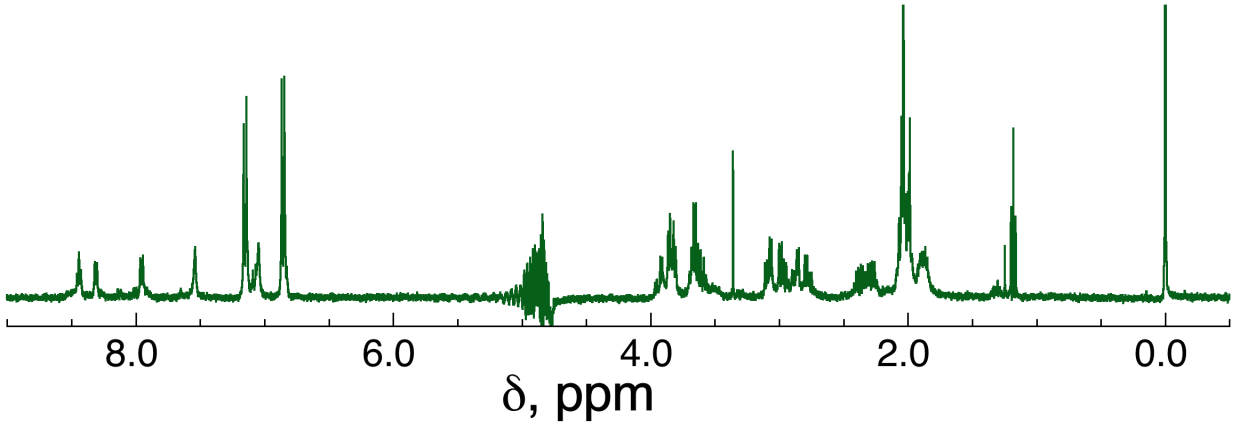


Figure S14. ^{1}H NMR spectrum of the peptide Ac-C(SO_3^-)-PPGY-NH_2 at 300 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

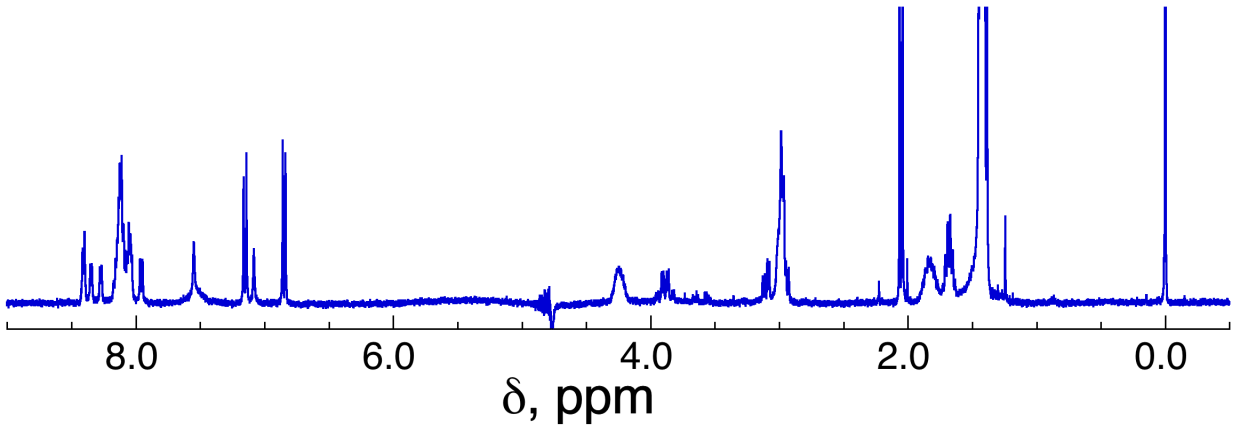


Figure S15. ^{1}H NMR spectrum of the peptide Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2 at 274 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

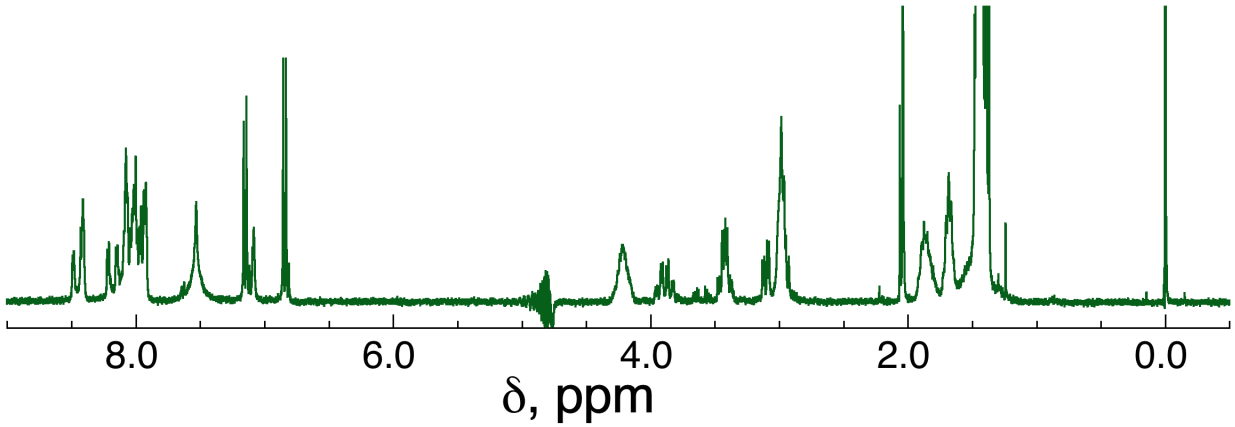


Figure S16. ^{1}H NMR spectrum of the peptide Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2 at 274 K in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

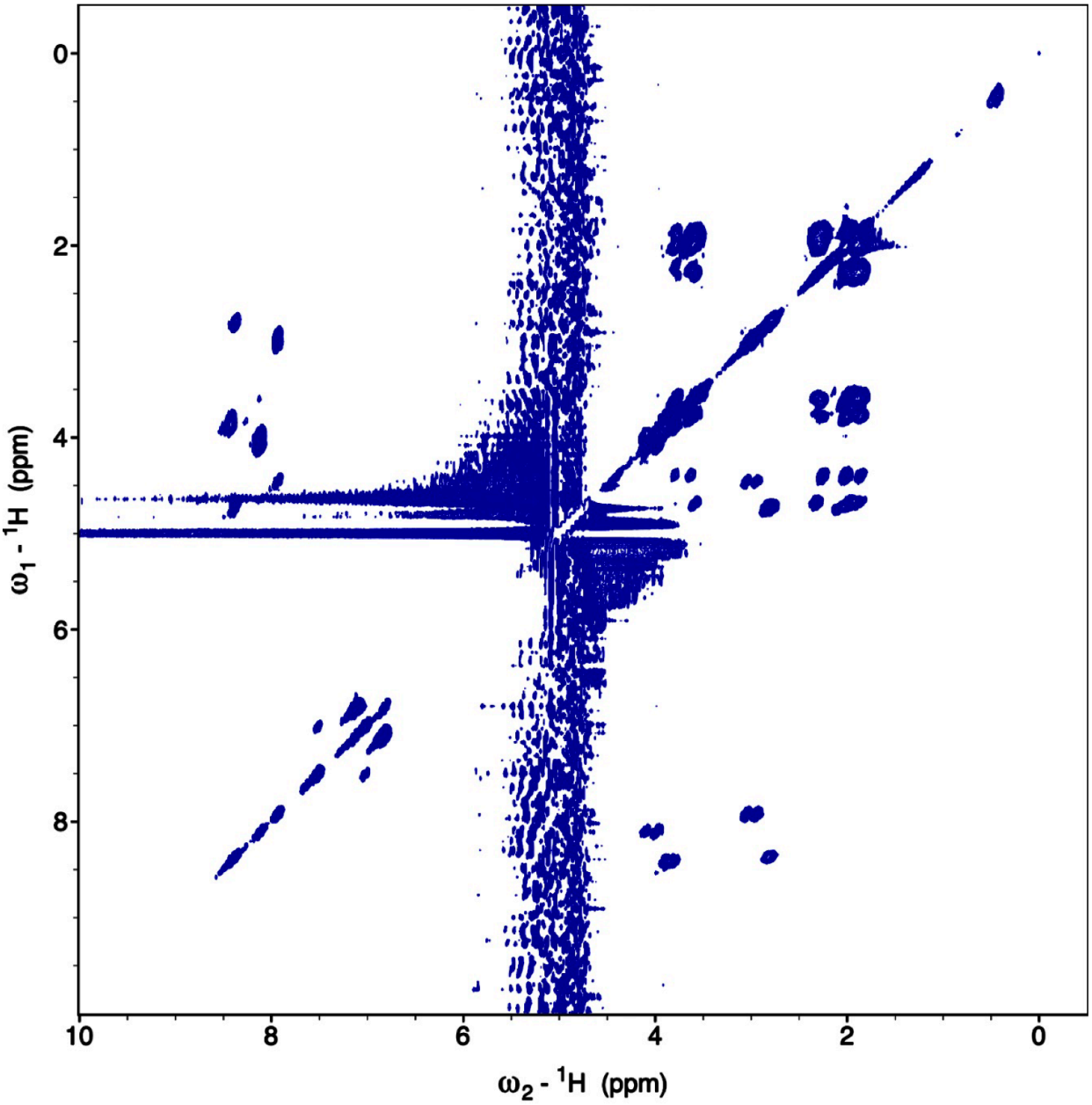


Figure S17. TOCSY NMR spectrum of Ac-GPP-C(SH)-PPGY-NH_2. Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

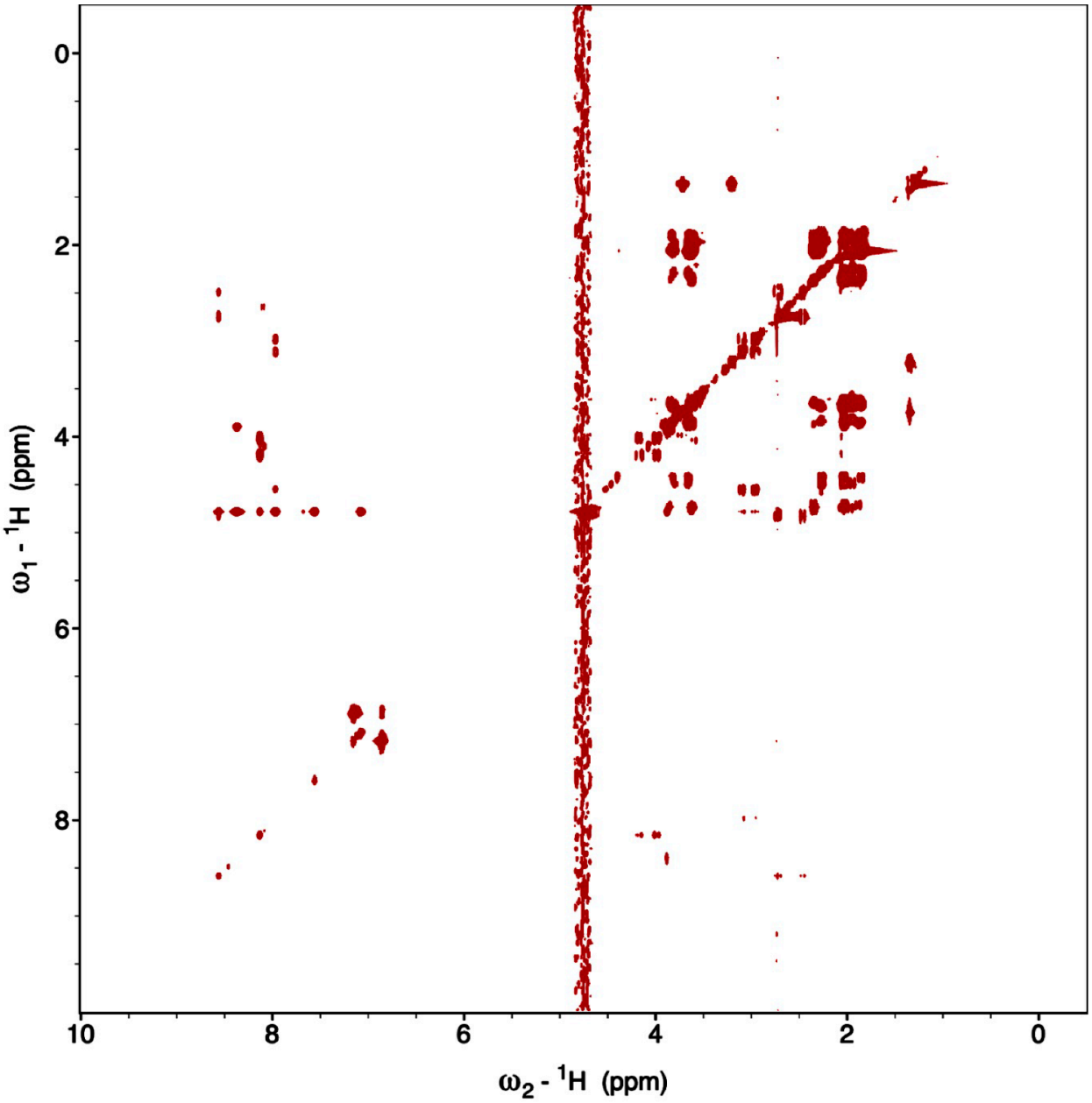


Figure S18. TOCSY NMR spectrum of Ac-GPP-C(SO_2^-)-PPGY-NH_2. Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

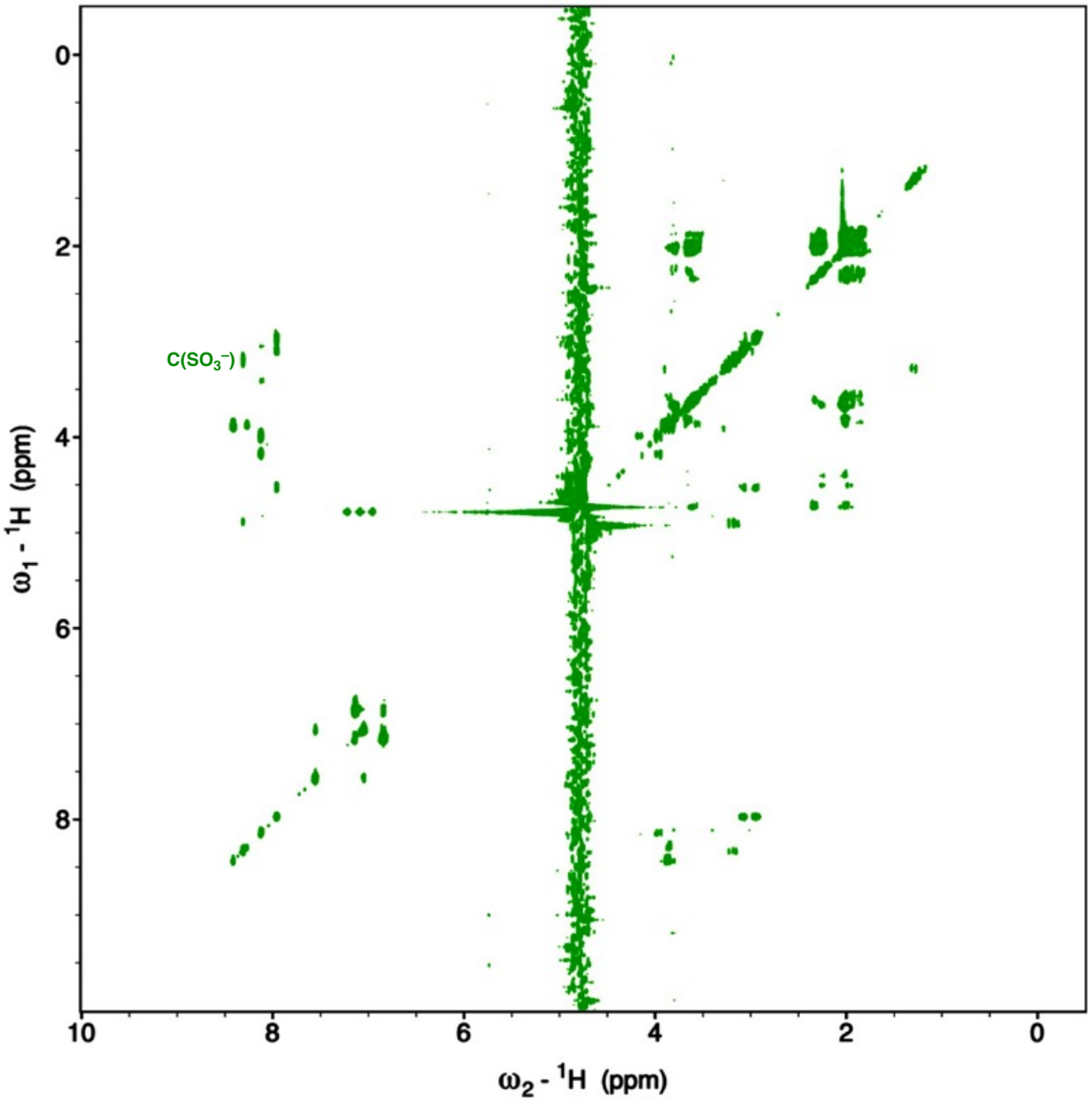


Figure S19. TOCSY NMR spectrum of Ac-GPP-C(SO_3^-)-PPGY-NH_2. Data were collected at 300 K on a Brüker AV 400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

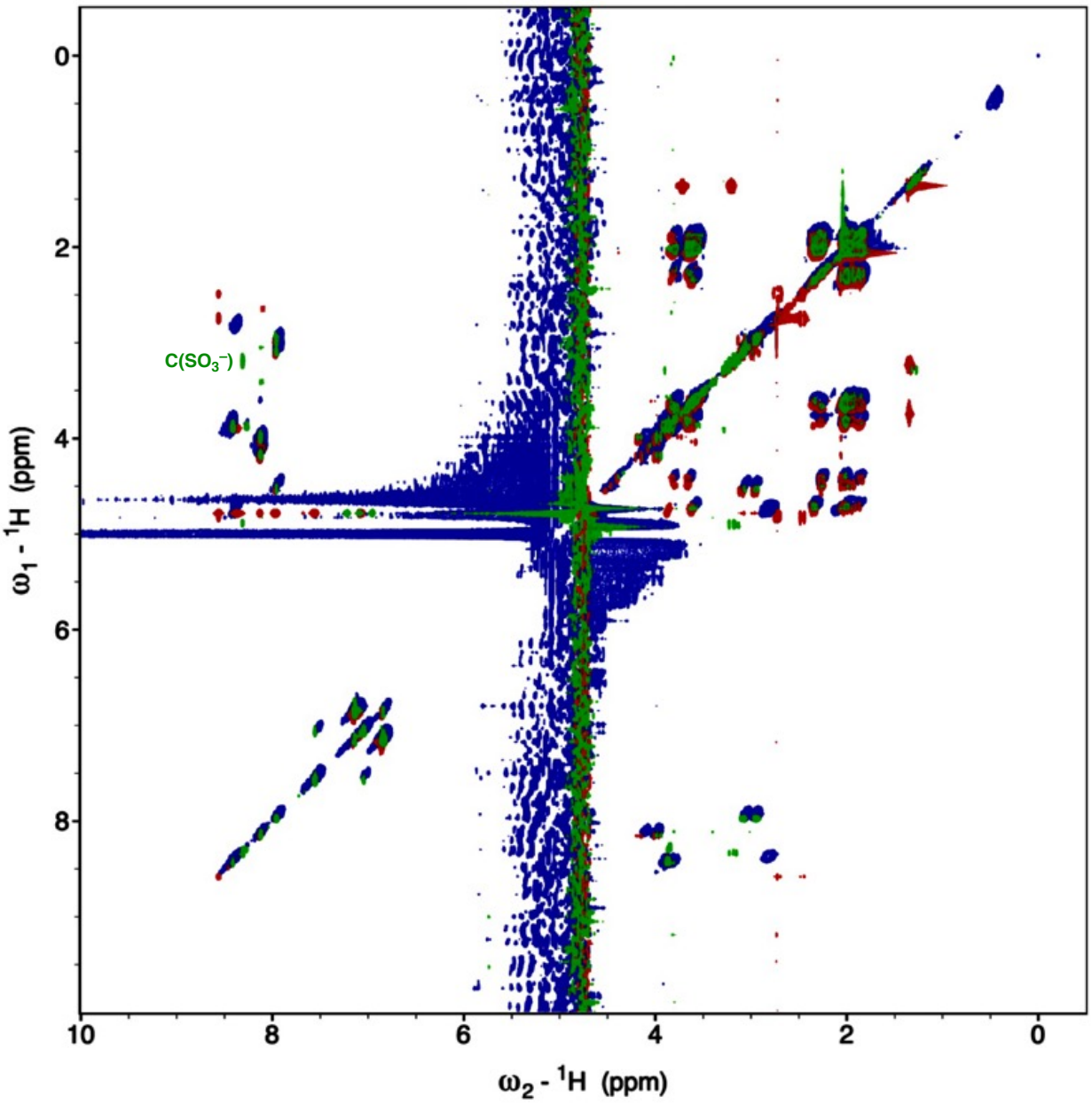


Figure S20. TOCSY NMR spectra of the peptides Ac-GPP-C(SH)-PPGY-NH_2, Ac-GPP-C(SO_2^-)-PPGY-NH_2[1], and Ac-GPP-C(SO_3^-)-PPGY-NH_2. Superposition of the TOCSY spectra of the peptides Ac-GPP-C(SH)-PPGY-NH_2 (blue), Ac-GPP-C(SO_2^-)-PPGY-NH_2 (red), and Ac-GPP-C(SO_3^-)-PPGY-NH_2 (green). Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

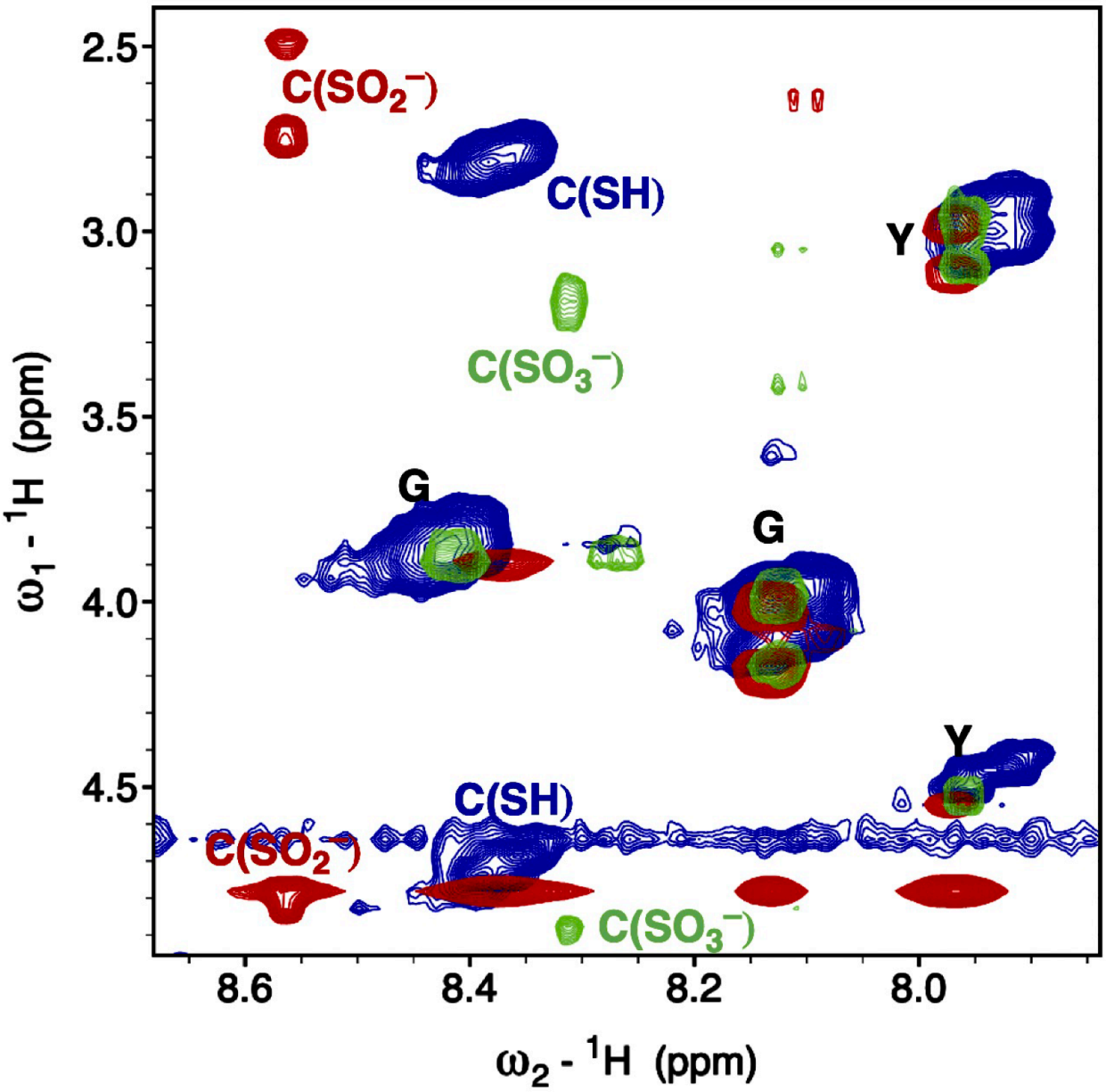


Figure S21. TOCSY NMR spectra (fingerprint region) of the peptides Ac-GPP-C(SH)-PPGY-NH_2, Ac-GPP-C(SO_2^-)-PPGY-NH_2, and Ac-GPP-C(SO_3^-)-PPGY-NH_2. Superposition of the TOCSY spectra of peptides Ac-GPP-C-(SH)-PPGY-NH_2 (blue), Ac-GPP-C(SO_2^-)-PPGY-NH_2 (red), and Ac-GPP-C-(SO_3^-)-PPGY-NH_2 (green). Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP. Assigned (major) peaks correspond to the peptides with all *trans*-proline amide bonds. Additional resonances are observed due to species with proline *cis* amide conformations.

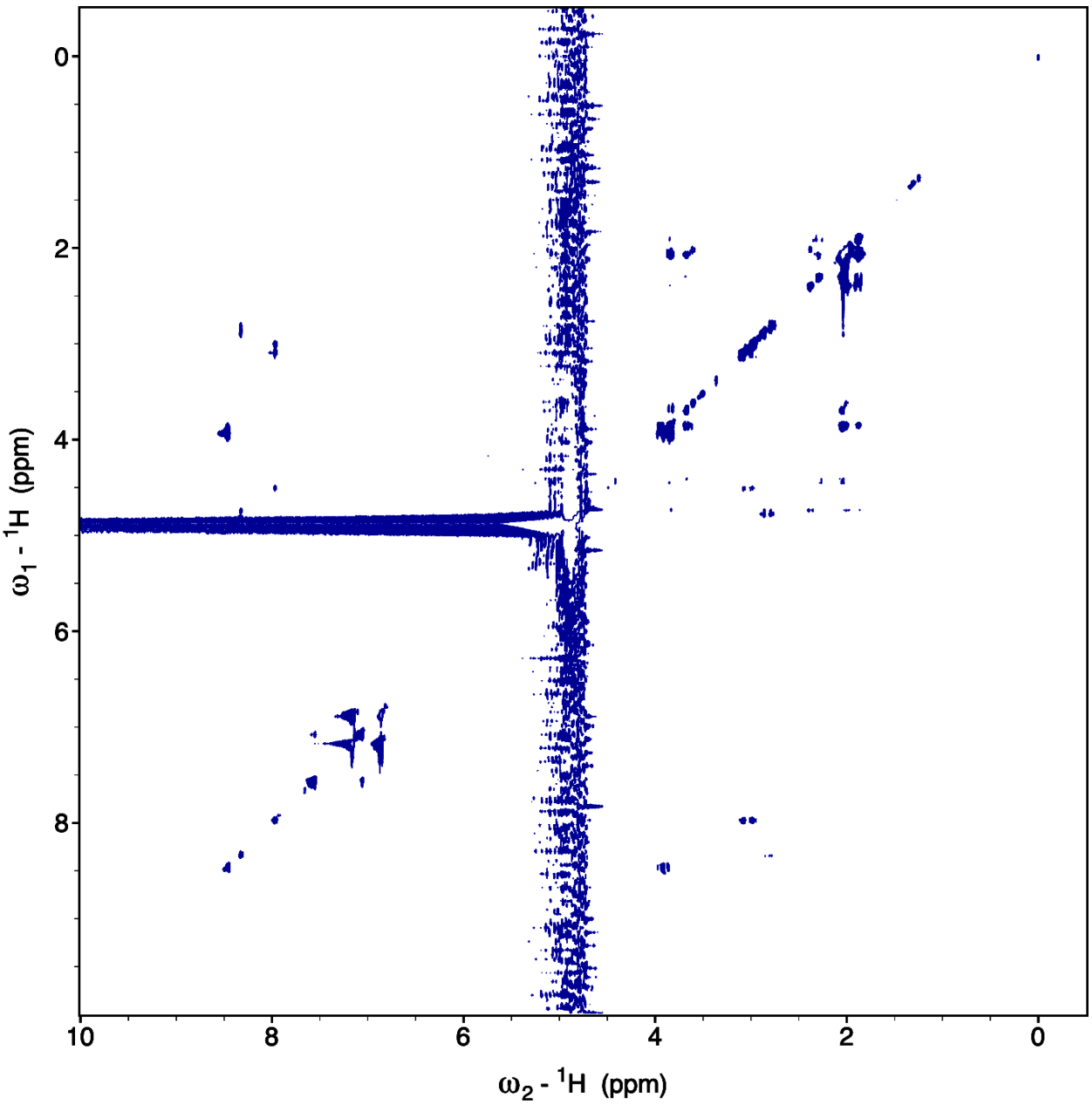


Figure S22. TOCSY NMR spectrum of Ac-C(SH)-PPGY-NH_2. Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptide in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

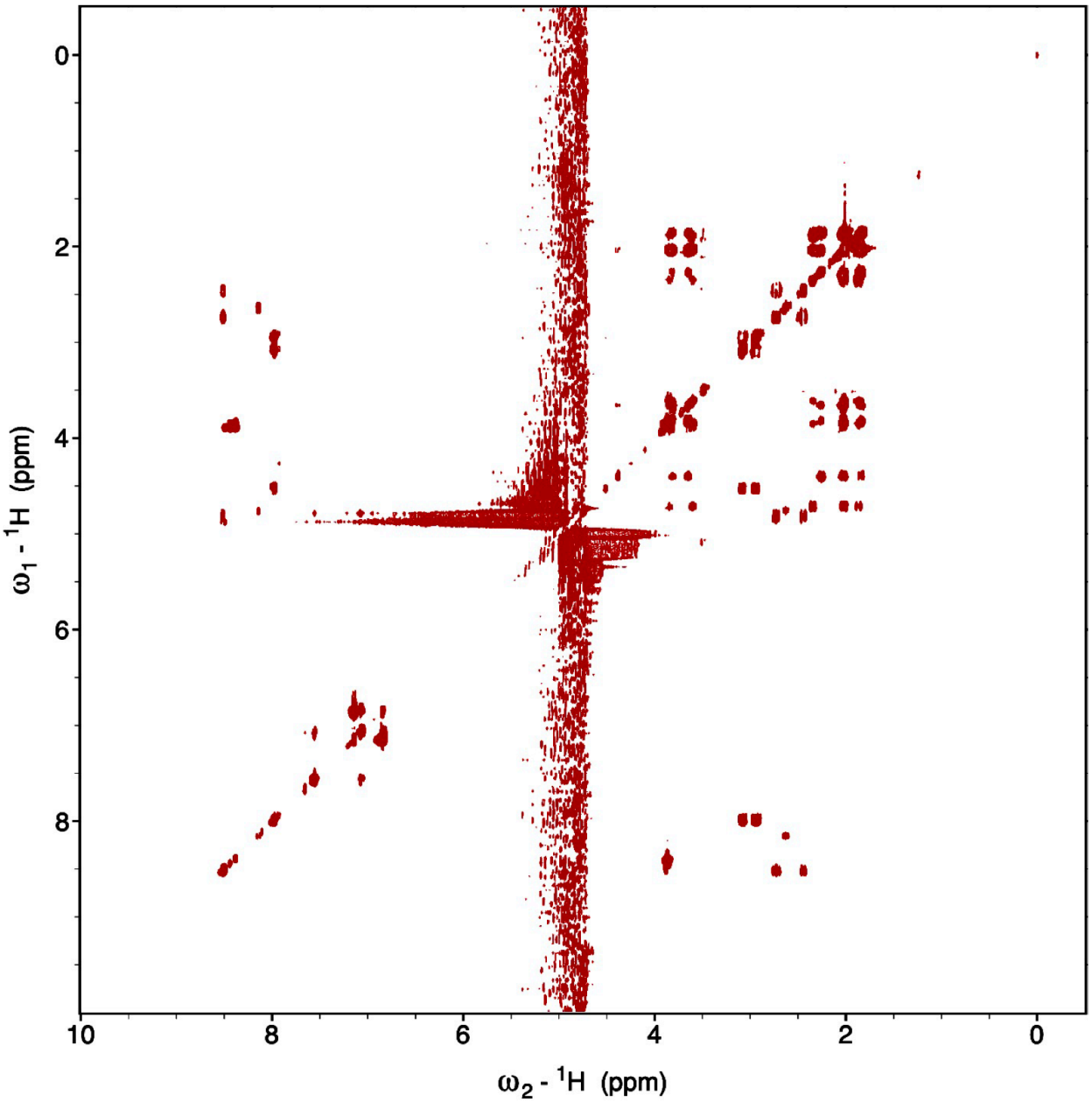


Figure S23. TOCSY NMR spectrum of Ac-C(SO_2^-)-PPGY-NH_2. Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

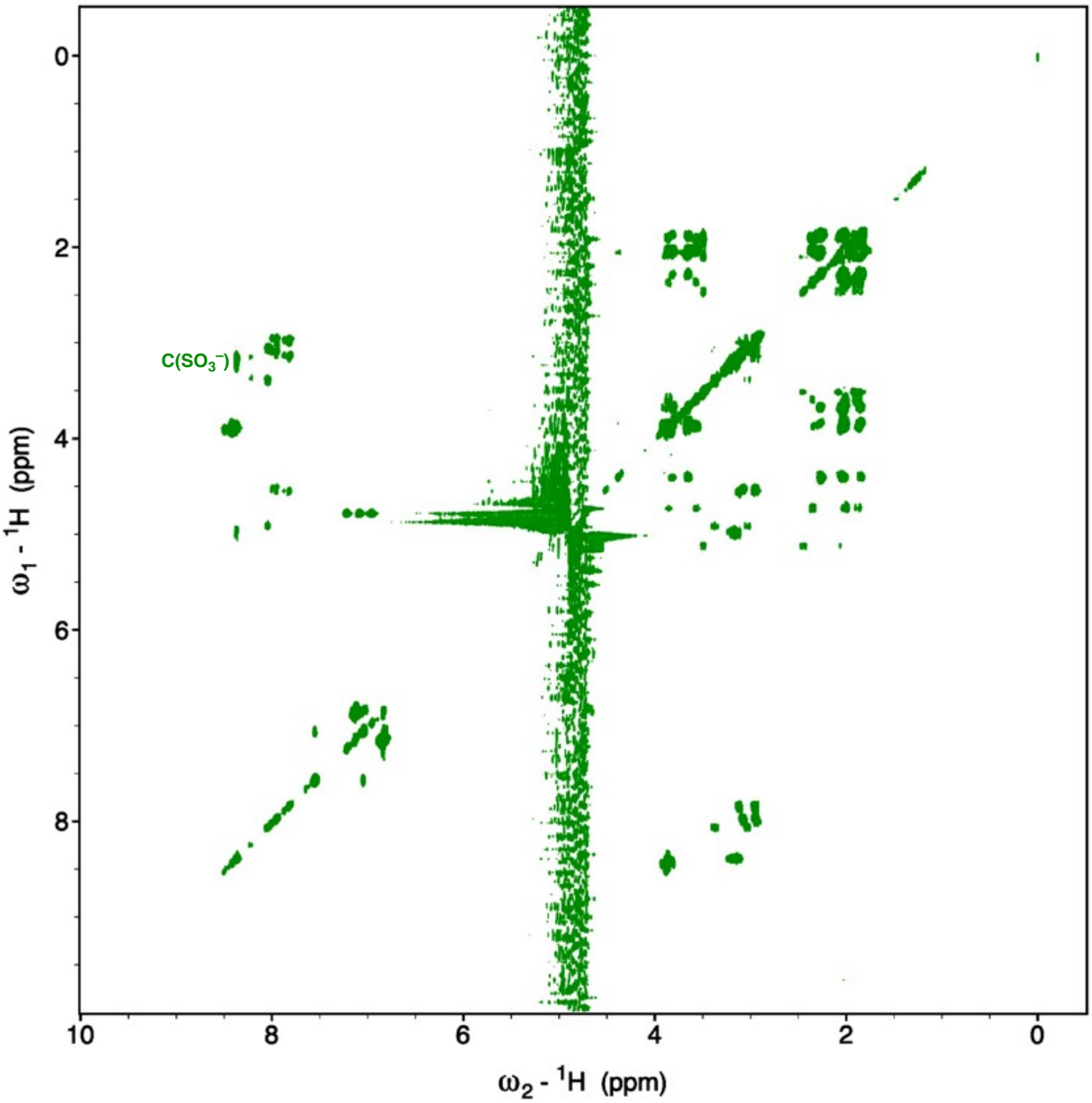


Figure S24. TOCSY NMR spectrum of Ac-C(SO_3^-)-PPGY-NH_2. Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

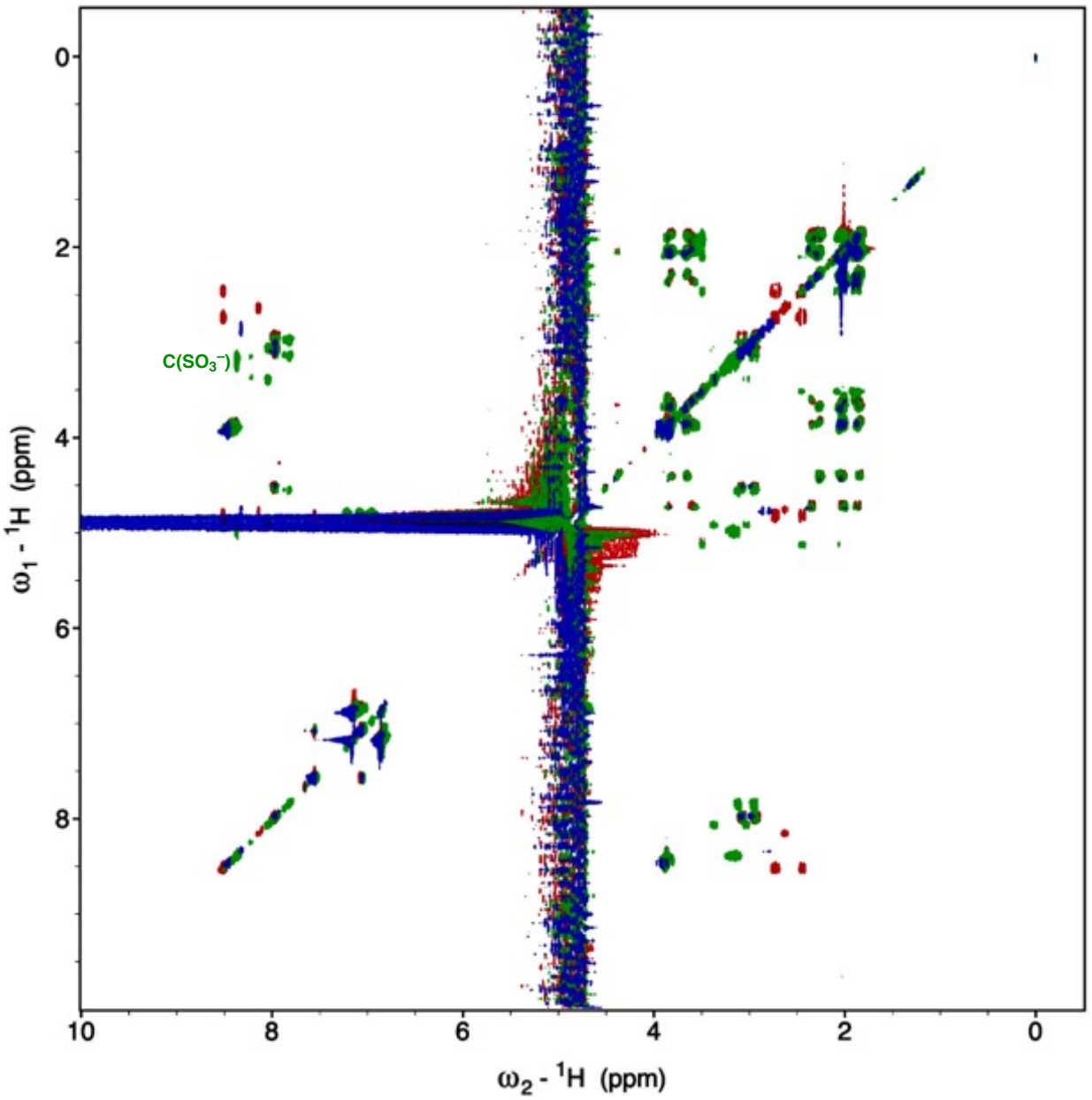


Figure S25. TOCSY NMR spectra of the peptides Ac-C(SH)-PPGY-NH_2, Ac-C(SO_2^-)-PPGY-NH_2, and Ac-C(SO_3^-)-PPGY-NH_2. Superposition of the TOCSY spectra of peptides Ac-C(SH)-PPGY-NH_2 (blue), Ac-C(SO_2^-)-PPGY-NH_2 (red), and Ac-C(SO_3^-)-PPGY-NH_2 (green). Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

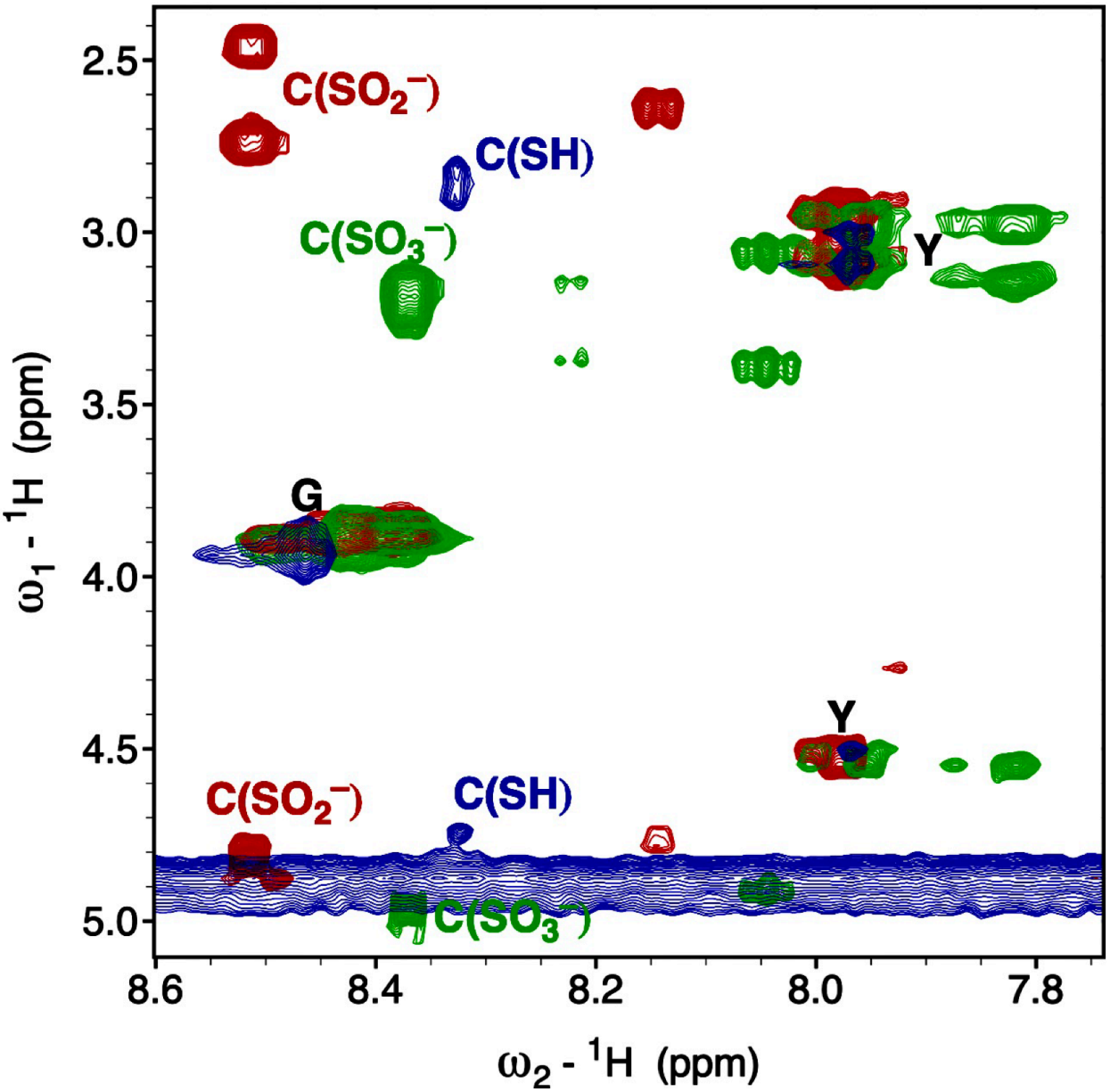


Figure S26. TOCSY spectra (fingerprint region) of the peptides Ac-C(SH)-PPGY-NH_2, Ac-C(SO_2^-)-PPGY-NH_2, and Ac-C(SO_3^-)-PPGY-NH_2. Superposition of the TOCSY spectra of peptides Ac-C(SH)-PPGY-NH_2 (blue), Ac-C(SO_2^-)-PPGY-NH_2 (red), and Ac-C(SO_3^-)-PPGY-NH_2 (green). Data were collected at 300 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP. Assigned (major) peaks correspond to the species with proline all-*trans* rotamers. Additional resonances are observed due to species with proline *cis* rotamers.

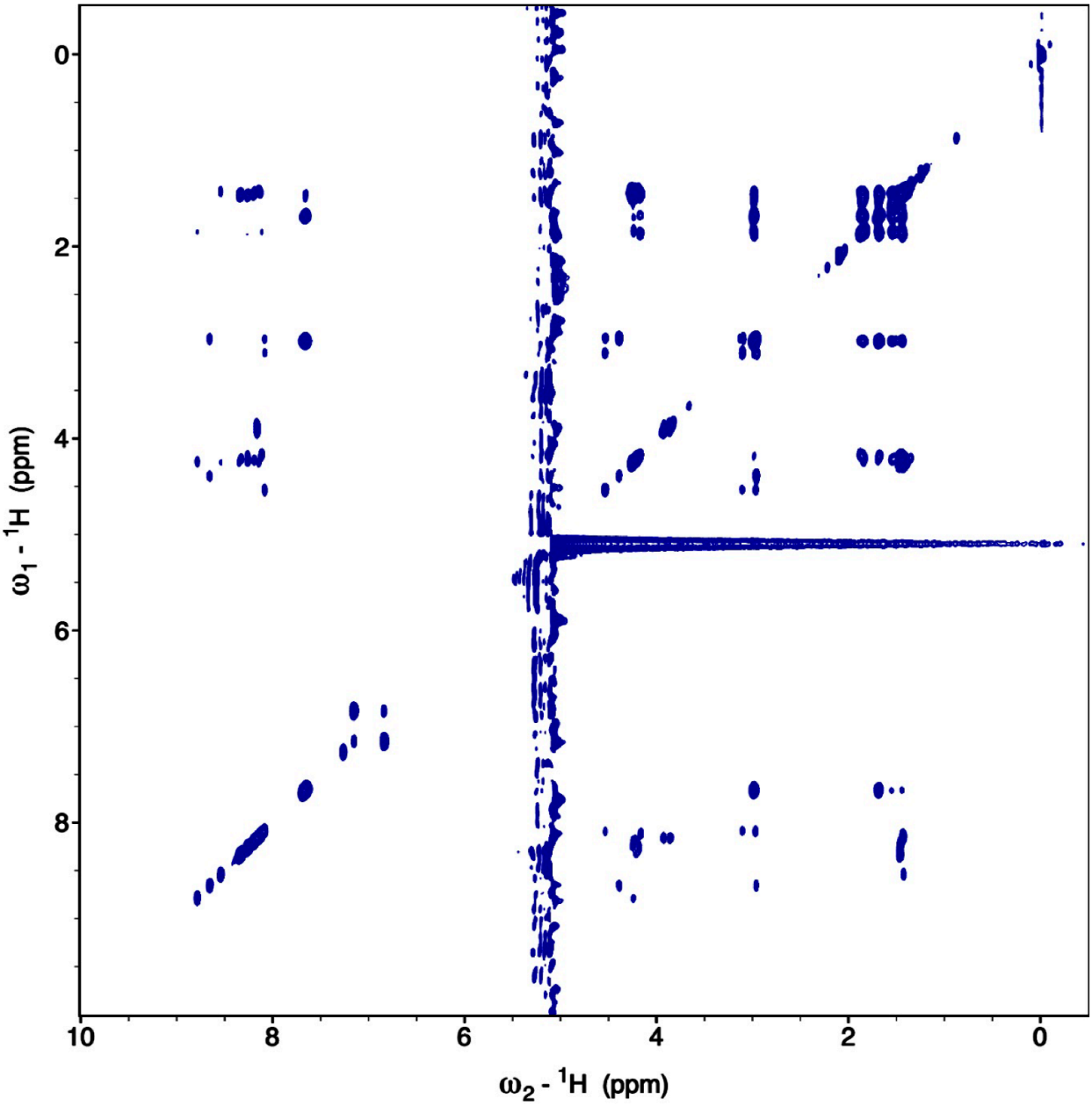


Figure S27. TOCSY NMR spectrum of Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2. Data were collected at 274 K on a Brüker AV400 MHz NMR spectrometer with the peptide in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 10 μM TSP.

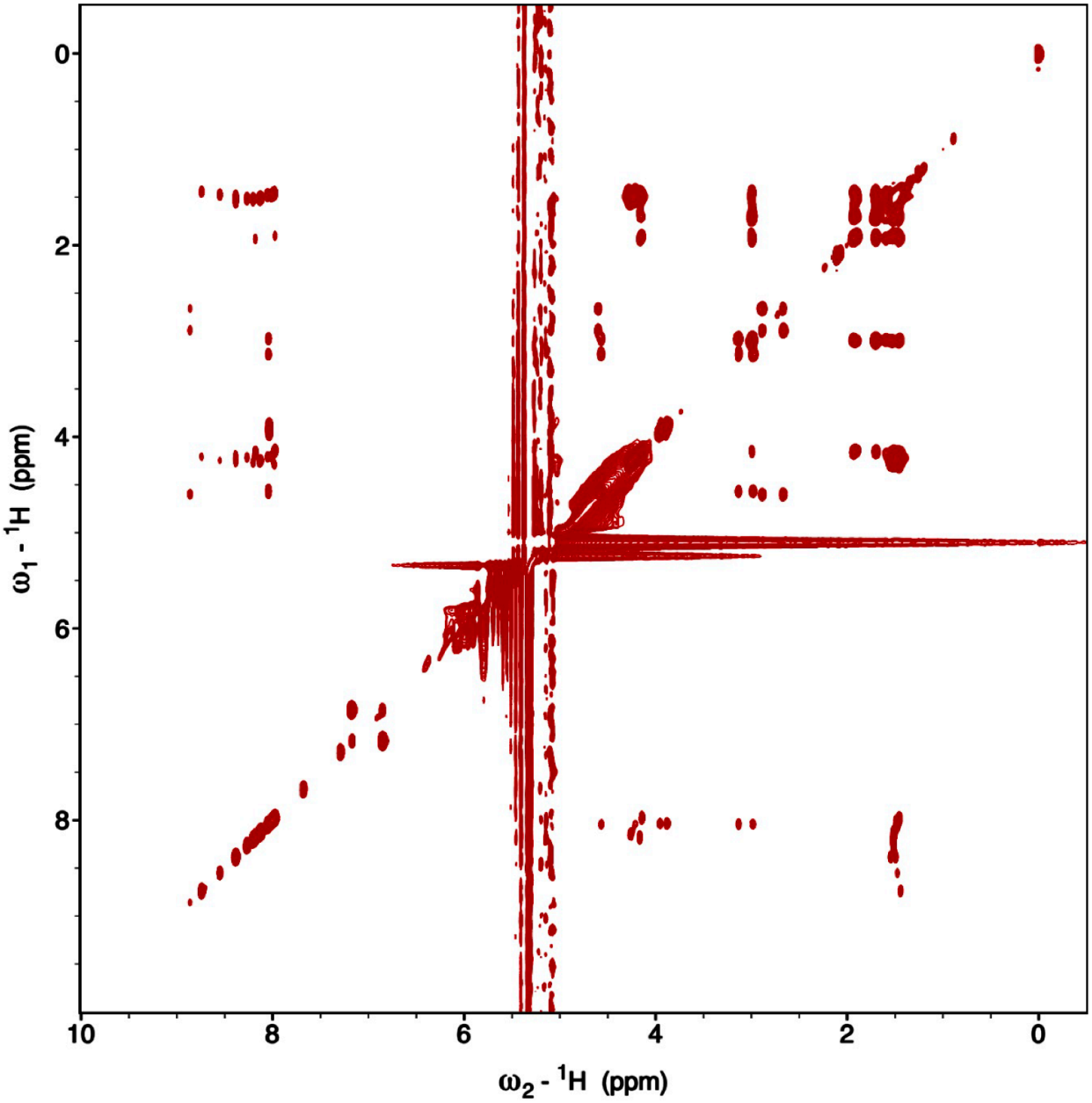


Figure S28. TOCSY NMR spectrum of Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2. Data were collected at 274 K on a Brüker AV400 MHz NMR spectrometer with the peptide in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

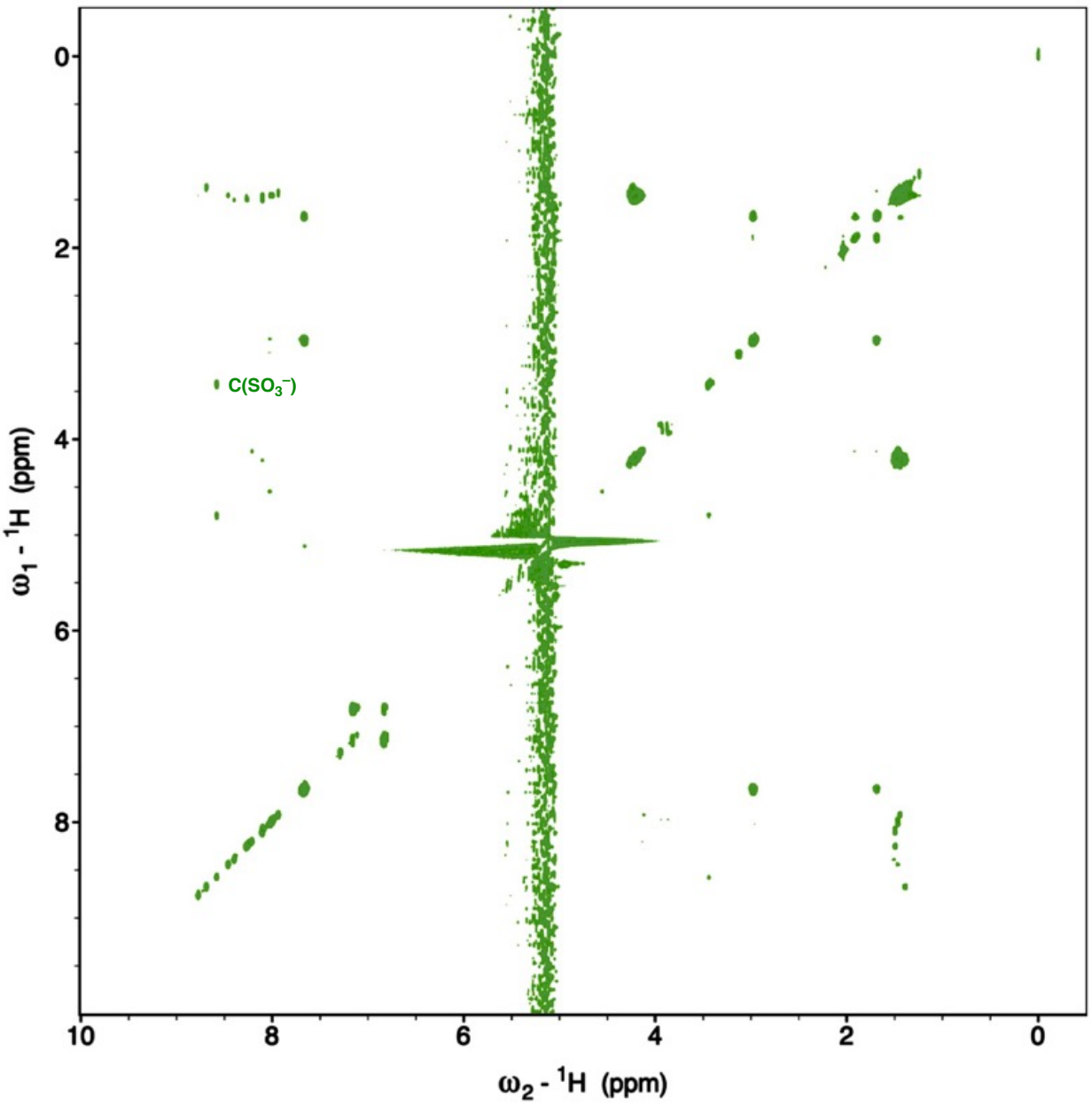


Figure S29. TOCSY NMR spectrum of Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2. Data were collected at 274 K on a Brüker AV400 MHz NMR spectrometer with the peptide in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

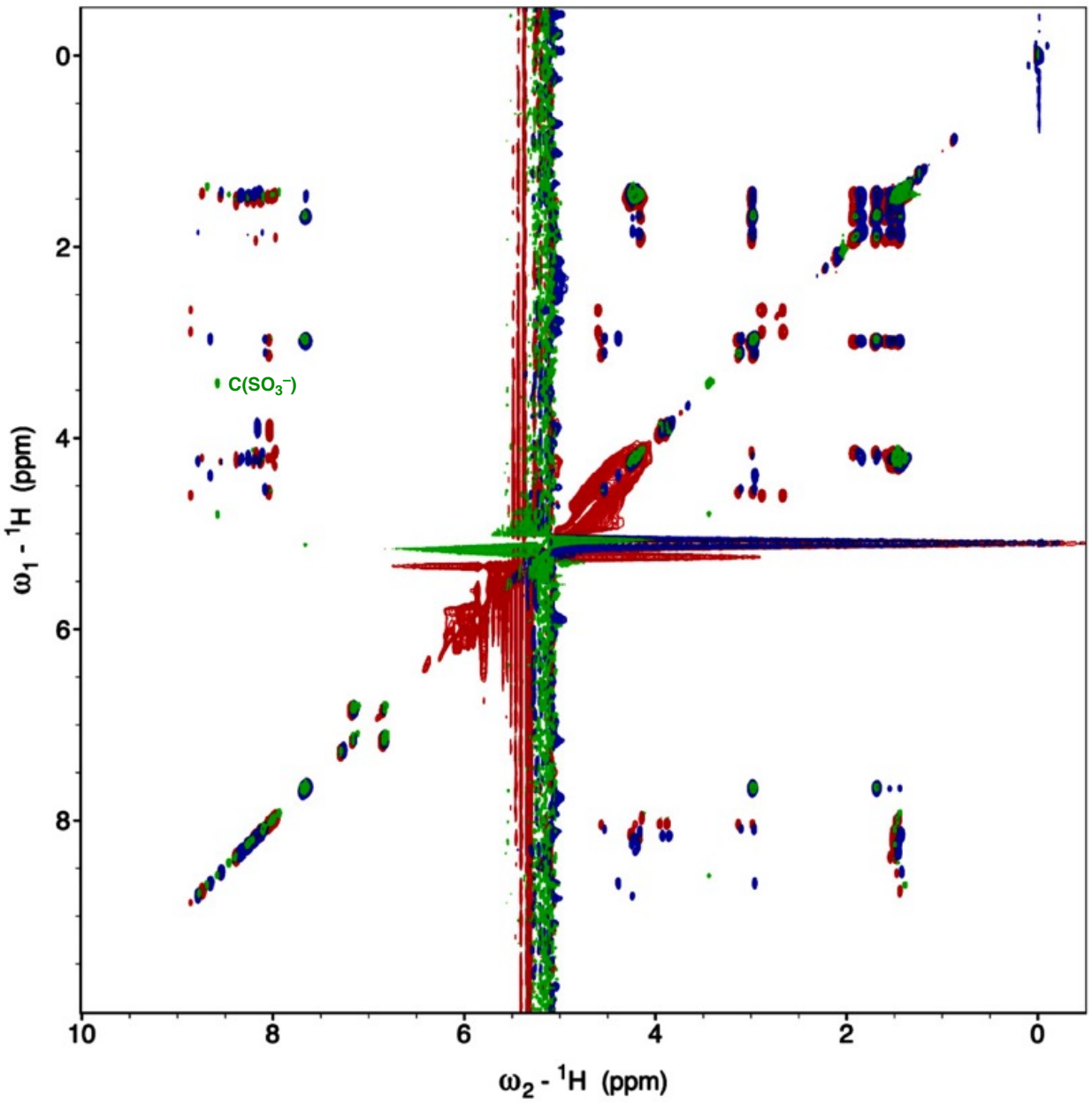


Figure S30. TOCSY NMR spectra of the peptides Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2[1], Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2[1], and Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2. Superposition of the TOCSY spectra of peptides Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2[1] (blue), Ac-AC-(SO_2^-)-AAAAKAAAAKAAGY-NH_2[1] (red), and Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2 (green). Data were collected at 274 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

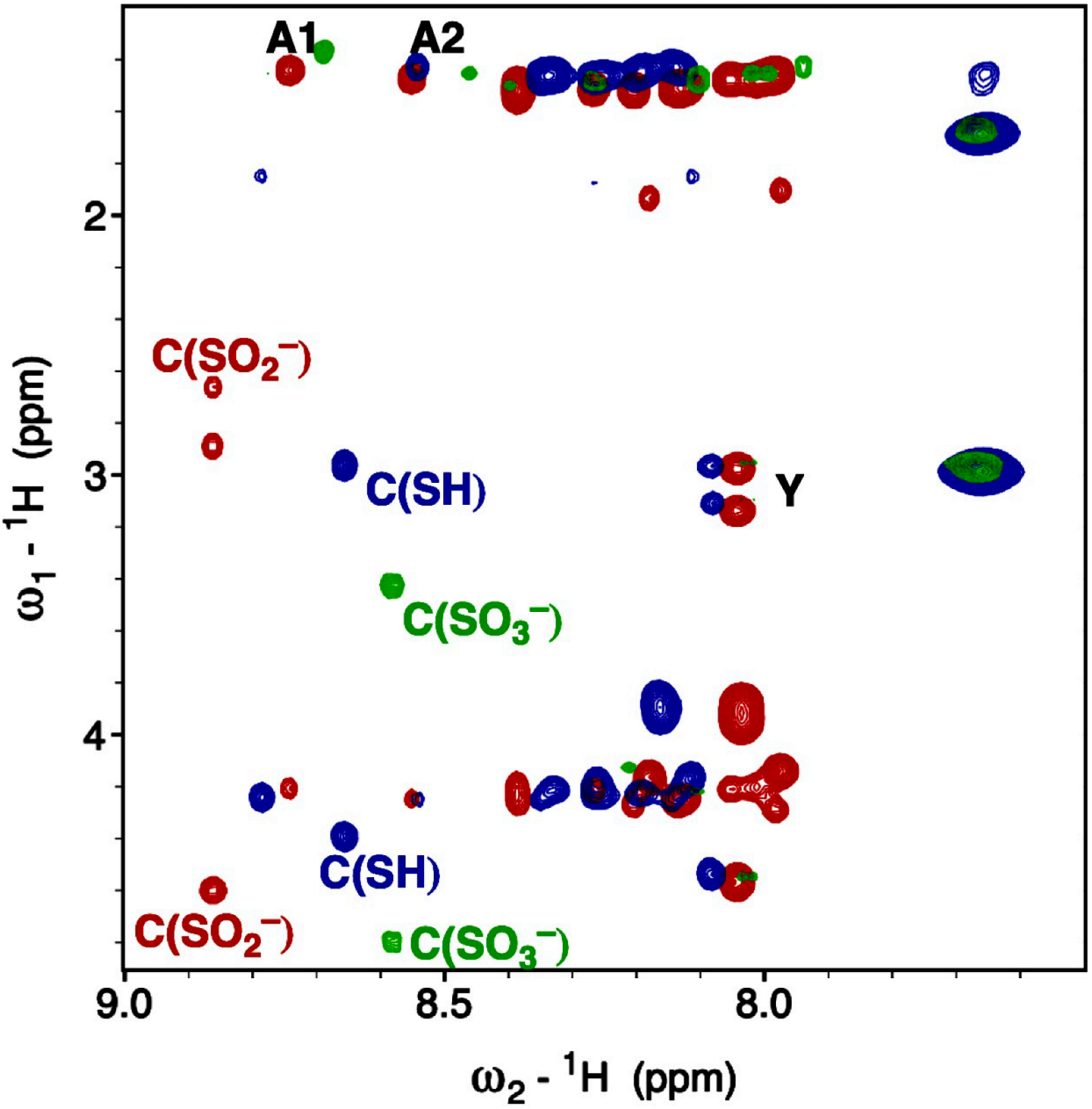


Figure S31. TOCSY NMR spectra (fingerprint region) of the peptides Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2[1], Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2[1], and Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2. Superposition of the TOCSY spectra of peptides Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2[1] (blue), Ac-AC-(SO_2^-)-AAAAKAAAAKAAGY-NH_2[1] (red), and Ac-A-C-(SO_3^-)-AAAAKAAAAKAAGY-NH_2 (green). Data were collected at 274 K on a Brüker AV400 MHz NMR spectrometer with the peptides in a solution of 90% H_2O/10% D_2O with 5 mM phosphate buffer pH 4 and 25 mM NaCl with 100 μM TSP.

Bioinformatics Analysis of Cysteine Sulfonic Acid, Cysteine Sulfinic Acid, and Cysteine

The Protein Data Bank (PDB) was investigated for structures containing cysteine sulfonic acid in a protein polymer (ligand ID OCS). On April 11, 2022, 146 cysteine sulfonic acid residues from 141 PDB structures at < 3.0 Å resolution with less than 90% sequence identity were obtained using the advanced search feature on the RCSB website. The text file (list_file.txt) with comma-separated PDB IDs was obtained from the above search, and corresponding PDB structure file in pdb format was downloaded using the batch-download shell script (batch_download.sh) obtained from the RCSB website. A text file (pdb-files-OCS.txt) with a single column list of PDB IDs of downloaded PDB files was created from the file "list_file.txt" by replacing the comma with a line break in a text editor. A perl script (sulfonate-finder.pl) was written to generate a text file "sulfonate-list.txt" containing a list of residues identified by PDB file name, chain ID, and residue number using the list of PDB IDs in file "pdb-files-OCS.txt" and respective PDB files in the same folder "OCS_PDB_project". An additional Perl script (sulfonate-harvester.pl) was written, which generated an output text file "OCS-structures.txt" containing parameters of the residues in the list using file "pdb-files-OCS.txt" and PDB files in the folder "OCS_PDB_project". The output file "OCS-structures.txt" contained the PDB ID, resolution, chain ID, residue number, structural annotation, identity, and main chain dihedral angles of the preceding residue, primary chain and side chain dihedral angles of Cys-SO_3^-, identity and main chain dihedral angles of the following residue, sulfonate sulfur-oxygen bond lengths, interatomic distances from each sulfonate oxygen to the preceding and the following amide nitrogen, interatomic distances from each sulfonate oxygen to the preceding and following amide carbonyl carbons, interatomic distances from the sulfonate sulfur to the preceding and following amide carbonyl carbons, and the carbonyl of the amide of the same residue (O---C=O angle), and the approximate Ramachandran region of the Cys-SO_3^- residue. Ramachandran regions were defined in the script, with the α-helical region defined as ($-110° \le \phi \le -30°$, $-80° \le \psi \le +30°$), the β/PPII region defined as ($\phi \le 0°$, $\psi \le -120°$ or $\psi \ge +60°$), the left-handed α-helical region defined as ($+30° \le \phi \le +110°$, $-30° \le \psi \le +80°$), and the right-handed PPII region defined as ($+30° \le \phi \le +90°$, $-180° \le \psi \le -90°$). The β and PPII regions were separated using Microsoft Excel. The β region was defined as ($-180° < \phi < -90°$ and [$\psi \le -120°$ or $+180° > \psi \ge +60°$]) and the PPII region defined as ($-90° \le \phi \le -40°$ and $+100° \le \psi \le +180°$). The resultant output file ("OCS-structures.txt") contains the data as tab-separated values suitable for opening and editing in Microsoft excel. Additional analysis was conducted within Microsoft Excel, including comparing interatomic distances to van der Waals radii graphs, and figures were generated using KaleidaGraph. The Perl scripts used in this study were adopted from a previous study from our group[1] and modified to make them suitable for this study. Structural data for 226 cysteine sulfinic acid residues (ligand ID CSD) from 216 PDB structures at < 3.0 Å resolution with less than 90% sequence identity were used to determine the backbone torsion angle preferences for cysteine sulfinic acid in proteins. Structural data for 1460 non-disulfide and unmodified cysteines (ligand ID CYS) from 431 PDB structures at ≤ 1.1 Å resolution with less than 30% sequence identity were used to determine the backbone torsion angle preferences for cysteine thiol/thiolate. The bioinformatics analysis was conducted on cysteine sulfinic acid (CSD) and cysteine (CYS) residues via a similar procedure as performed for the study of cystine sulfonic acid (OCS).

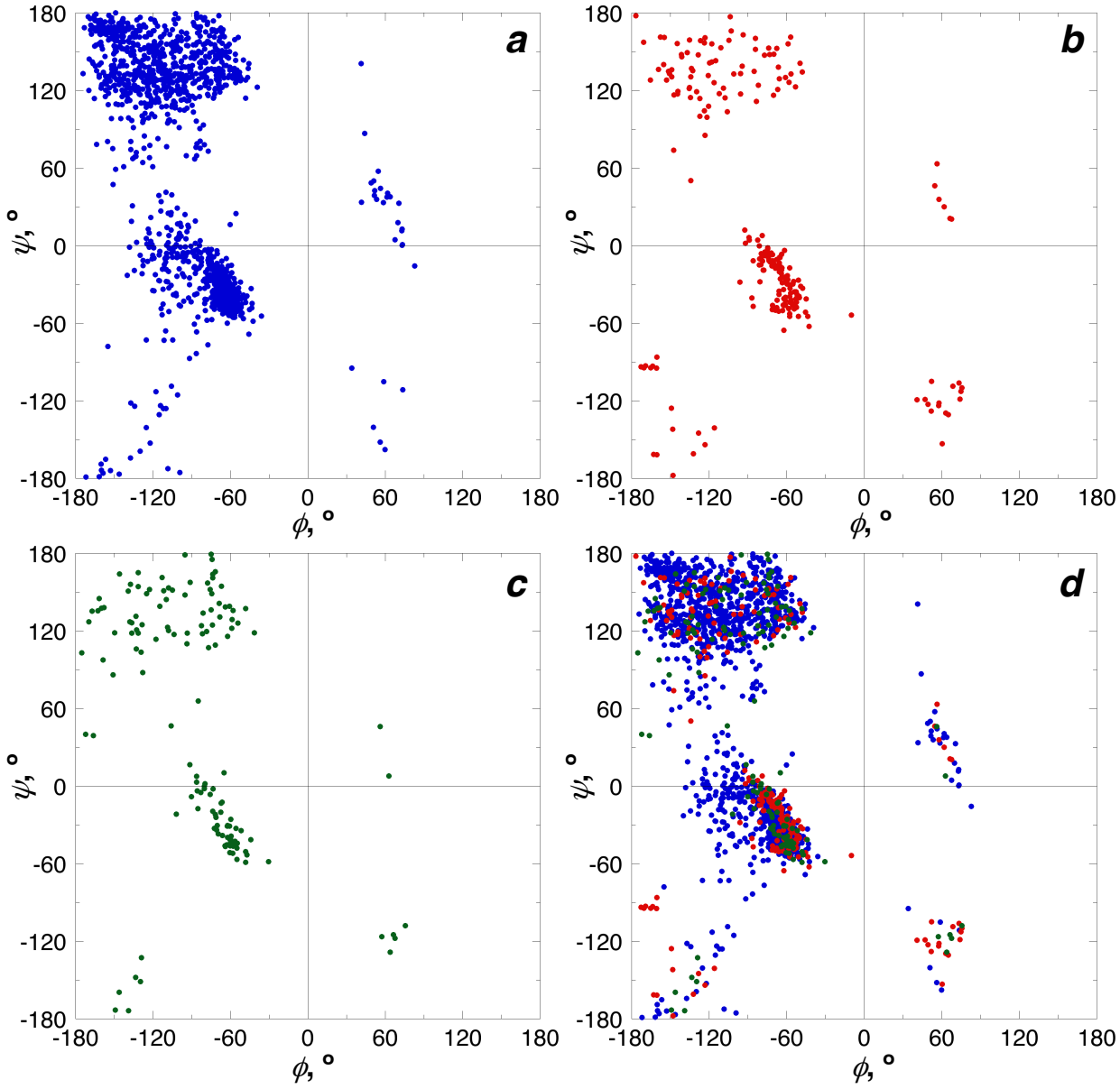


Figure S32. Ramachandran plots of cysteine, cysteine sulfinic acid, and cysteine sulfonic acid residues in the PDB**.** Ramachandran plot of (a) cysteine, (b) cysteine sulfinic acid, and (c) cysteine sulfonic acid residues in the PDB. (d) superimposition of Ramachandran plots of cysteine (blue), cysteine sulfinic acid (red), and cysteine sulfonic acid (green) residues in the PDB.

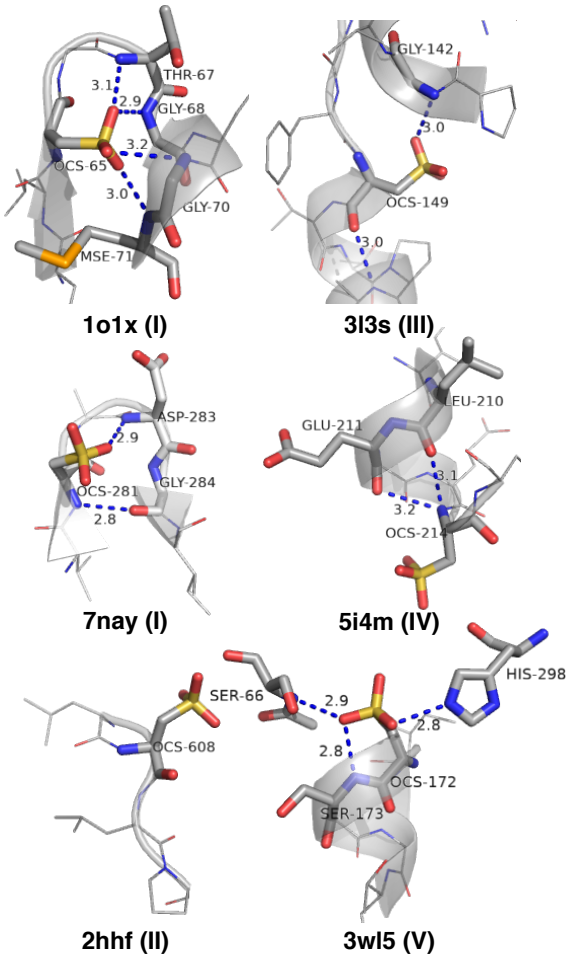


Figure S33. Representative Cys-SO_3^- residues (OCS) in PDB structures in different quadrants of the Ramachandran plot (Figure 13b), as indicated by Roman numerals. In PDB 1o1x, the cysteine sulfonic residue (OCS-65) is present near the loop, forming torsional angles ϕ –139º, ψ –174º, and χ_1 +70º. Two of the oxygen atoms of Cys-SO_3^- form hydrogen bonds with amide nitrogens of residues Thr-67, Gly-68, Gly-70, and Mse-71. In PDB 7nay, the cysteine sulfonic acid (OCS-281) is present near the loop, forming torsional angles ϕ –149º, ψ –173º, and χ_1 +61º. One of the oxygens of Cys-SO_3^- forms hydrogen bonds with the amide nitrogen of residue Asp-283. In PDB 2hhf, the cysteine sulfonic acid (OCS-608) is present in a loop, forming torsional angles ϕ –172º, ψ +40º, and χ_1 –148º. The oxygen atoms of Cys-SO_3^- don't interact with any of the backbone atoms. In PDB 3l3s, the cysteine sulfonic acid (OCS-149) is present near the N-terminus of an α-helix, forming torsional angles ϕ –85º, ψ +65º, and χ_1 –83º. One of the oxygens of Cys-SO_3^- interacts with the amide nitrogen of (Gly-142), forming a hydrogen bond. In PDB 4i4m, the cysteine sulfonic acid (OCS-214) is present near the C-terminus of an α-helix, forming torsional angles ϕ 56º, ψ 46º, and χ_1 –80º. The oxygens of Cys-SO_3^- don't interact with any of the backbone atoms. In PDB structure 3wl5, the cysteine sulfonic acid (OCS-172) is present near the N-terminus of an α-helix forming, torsional angles ϕ; +64º, ψ; –128º, and χ_1; –176º. One of the oxygens of Cys-SO_3^- forms dual hydrogen bonds with the amide nitrogens of residues Ser-66 and Ser-173, while another oxygen forms a single hydrogen bond with the amide nitrogen of residue His-298.

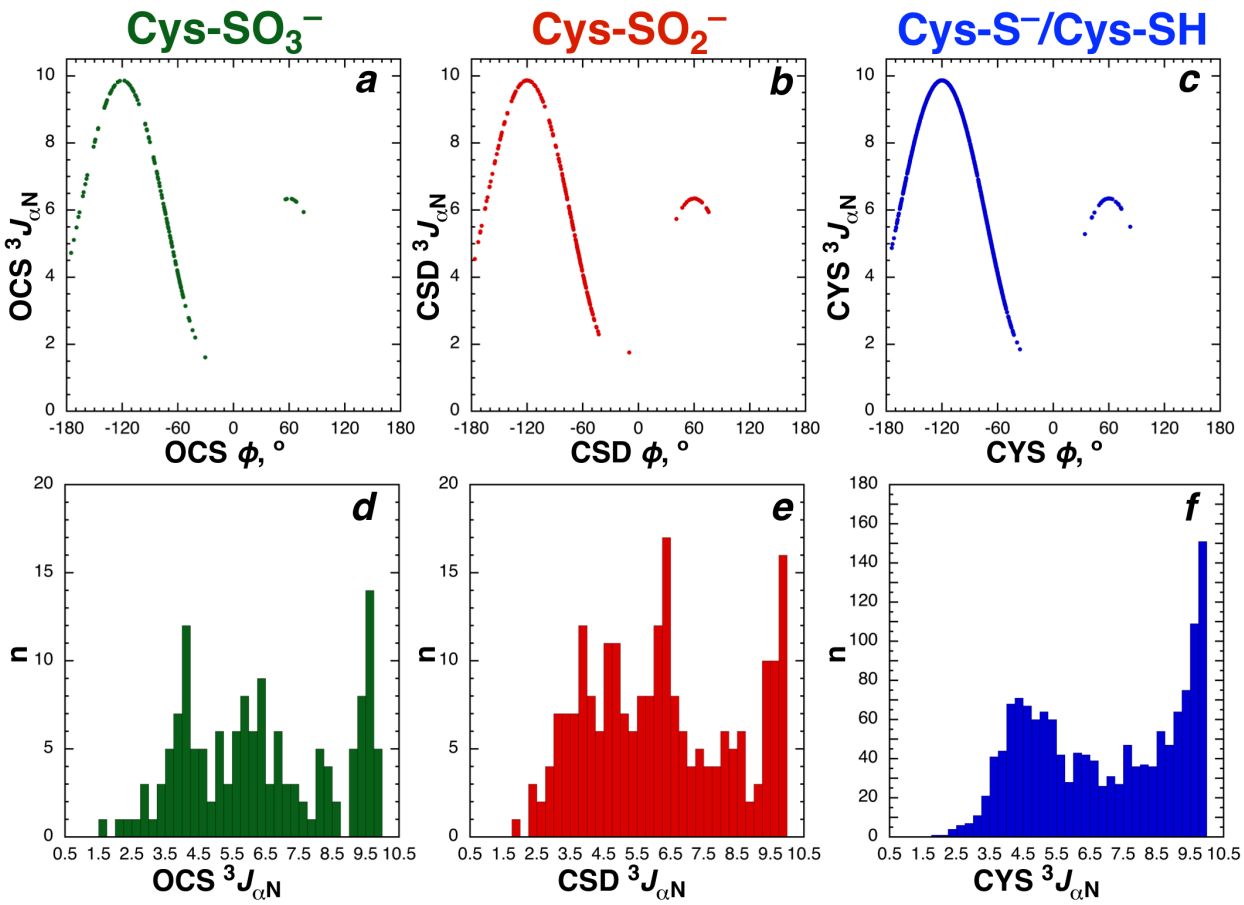


Figure S34. Karplus relationship of the $^{3}J_{\alpha N}$ coupling constants calculated from the observed ϕ dihedral angle in cysteine sulfonate, cysteine sulfinate, and cysteine in PDB structures. The subfigures (a), (b), and (c) represent the Karplus curve of the $^{3}J_{\alpha N}$ coupling constants in cysteine sulfinate, cysteine sulfonate, and cysteine respectively, in PDB structures. The subfigures (d), (e), and (f) represent histograms of the Karplus relationship of the $^{3}J_{\alpha N}$ coupling constants in cysteine sulfinate, cysteine sulfonate, and cysteine respectively, in PDB structures. The average Karplus constant was found to be 6.34 Hz for Cys-SO_3^-, 6.32 Hz for Cys-SO_2^-; and 6.89 Hz for Cys-S^-/Cys-SH. The smaller $^{3}J_{\alpha N}$ in the case of Cys-SO_3^- and Cys-SO_2^- residues indicate their ability to promote more compact conformations (α-helix) than that promoted by cysteine. The Karplus constants were calculated using the Karplus equation: $^{3}J_{HN\alpha} = 6.5 \cos^2(\phi - 60^{o}) - 1.76 \cos(\phi - 60^{o}) + 1.6$, where ϕ is the observed ϕ dihedral angle of respective cysteine oxoforms in the PDB structures.

residue	calculated $^3J_{\alpha N}$				total
	1–4.5	4.5–7.5	7.5–10	average	residues
	40	60	46		146
Cys-SO_3^-	27.4%	41.1%	31.5%	6.34	
	57	103	66		226
Cys-SO_2^-	25.2%	45.6%	29.2%	6.32	
	273	531	656		1460
Cys	18.7%	36.4%	44.9%	6.89	

Table S5. Summary of the Karplus values of the $^3J_{\alpha N}$ coupling constants in cysteine sulfonate, cysteine sulfinate, and cysteine in the structures from the PDB from Figure S34. All measurements were performed using the Perl script and analyzed using Microsoft Excel. The Karplus constants were calculated using the Karplus equation: $^3J_{\alpha N} = 6.5 \cos^2(\phi - 60^o) - 1.76 \cos(\phi - 60^o) + 1.6$, where ϕ is the observed ϕ dihedral angle of respective cysteine oxoforms in the PDB structures.

Residue	$-180^o \le \phi^o < -110^o$ %	$-110^o \le \phi^o < -30^o$ %	$-30^o \le \phi^o < +30^o$ %	$+30^o \le \phi^o < +110^o$ %	$+110^o \le \phi^o < +180^o$ %
Cys-SO_3^-	26.7	68.5	0.0	4.8	0.0
Cys-SO_2^-	27.9	62.4	0.4	9.3	0.0
Cys	32.9	65.1	0.0	1.9	0.0

Table S6. Summary of ϕ dihedral angles of cysteine sulfonic acid, cysteine sulfinic acid, and cysteine residues in the PDB.

Residue	$-180^o \le \psi^o < -110^o$ %	$-110^o \le \psi^o < -30^o$ %	$-30^o \le \psi^o < +30^o$ %	$+30^o \le \psi^o < +110^o$ %	$+110^o \le \psi^o < +180^o$ %
Cys-SO_3^-	6.8	26.7	15.1	9.6	41.8
Cys-SO_2^-	8.8	26.5	27.9	4.9	31.9
Cys	1.8	30.0	15.2	6.3	46.7

Table S7. Summary of ψ dihedral angles of cysteine sulfonic acid, cysteine sulfinic acid, and cysteine residues in the PDB.

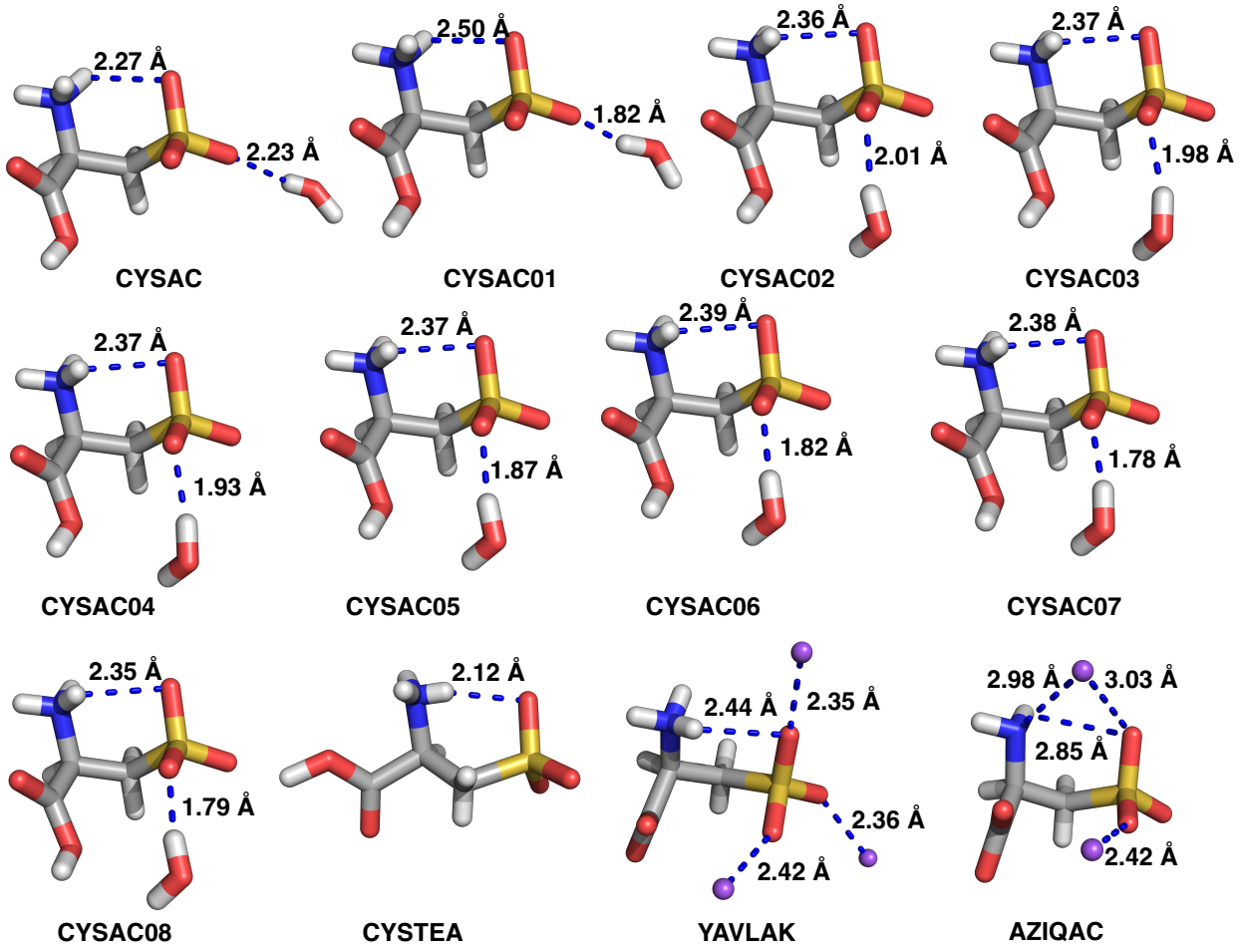


Figure S35. Crystal structures of cysteine sulfonate in the Cambridge Structural Database (CSD). The structures are shown with CSD identifiers. All the distances are measured after hydrogen position normalization in Mercury. In the case of CYSTEA, where no water molecule is present, the SO_3^-•••NH hydrogen bond is closest (2.12 Å). In the presence of water molecules, it is observed that a stronger SO_3^-•••OH_2 hydrogen bond formed by any one oxygen of Cys-SO_3^- weakens the SO_3^-•••NH bond formed by another oxygen of Cys-SO_3^-. These results suggest that the solvation of cysteine sulfonic acid residue in peptide weakens the strength of (SO_3^-•••NH) hydrogen bond with backbone amide hydrogen. The structure AZIQAC shows that Na^+ ions can form a salt bridge (SO_3^-••Na^+••NH).

CSD entry	reference	SO_3^-••Na^+ d, Å	SO_3^-••NH d, Å	SO_3^-••HOH d, Å	ψ^o	χ_1
CYSTAC	[2]	-	2.27	2.23	–169	+56
CYSTAC01	[3]	-	2.50	1.82	–169	+56
CYSTAC02	[4]	-	2.36	2.01	–170	+55
CYSTAC03	[4]	-	2.37	1.98	–170	+55
CYSTAC04	[4]	-	2.37	1.93	–170	+55
CYSTAC05	[4]	-	2.37	1.87	–170	+55
CYSTAC06	[4]	-	2.39	1.82	–168	+55
CYSTAC07	[4]	-	2.38	1.78	–167	+54
CYSTAC08	[4]	-	2.35	1.79	–166	+54
CYSTEA	[5]	-	2.12	-	–9	–75
YAVLAK	[6]	2.35, 2.36, 2.42	2.44	-	N/A	+56
AZIQAC	[7]	2.42	2.85	N/A	N/A	+56

Table S9. Summary of crystal structures of cysteine sulfonate in the CSD (see Figure S35). The structures are shown with CSD identifiers. All measurements were performed after hydrogen position normalization in Mercury.

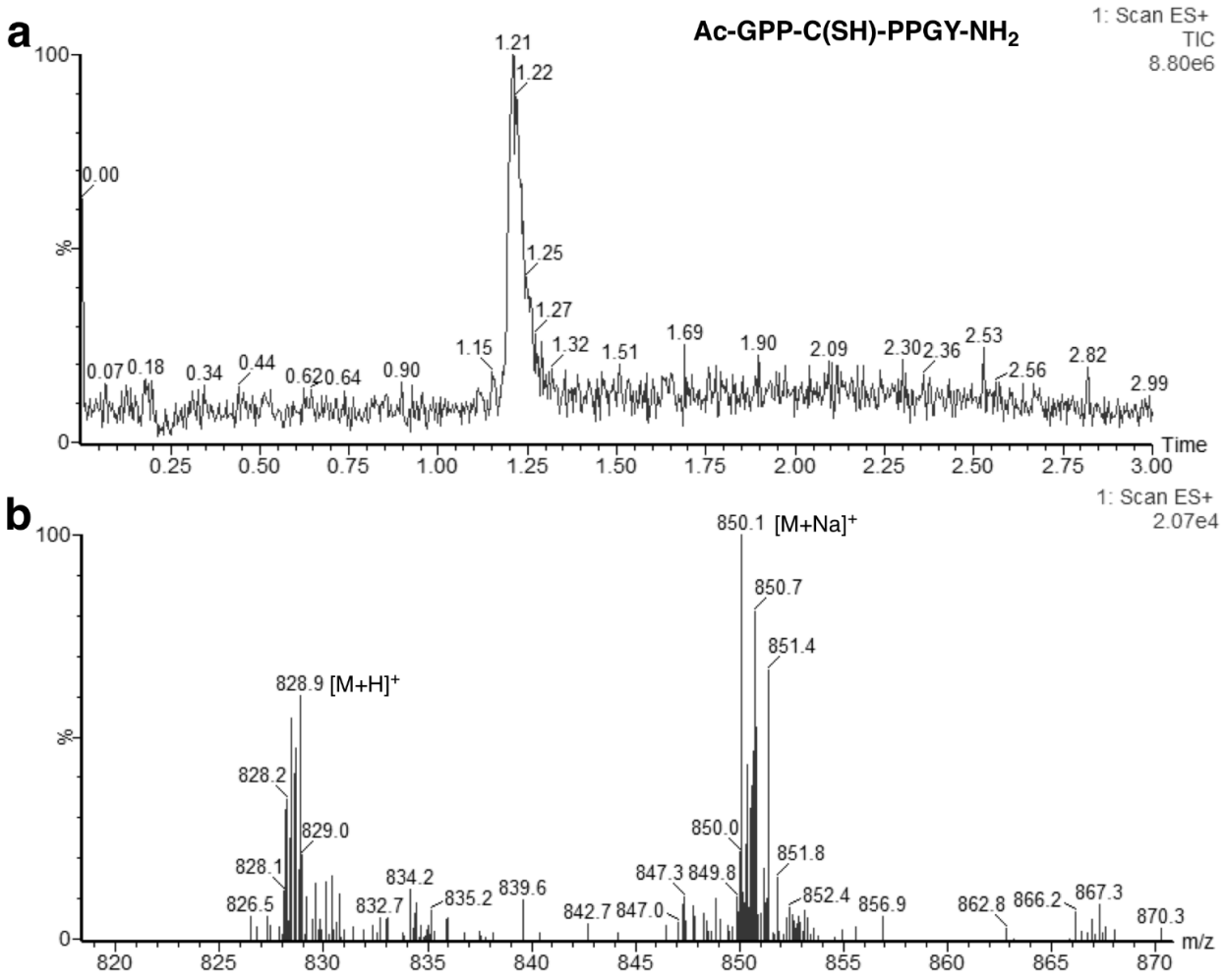


Figure S36. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-GPP-C(SH)-PPGY-NH_2. Calculated exact mass: 827.4; observed: 828.9 $[M+H]^+$, 850.1 $[M+Na]^+$.

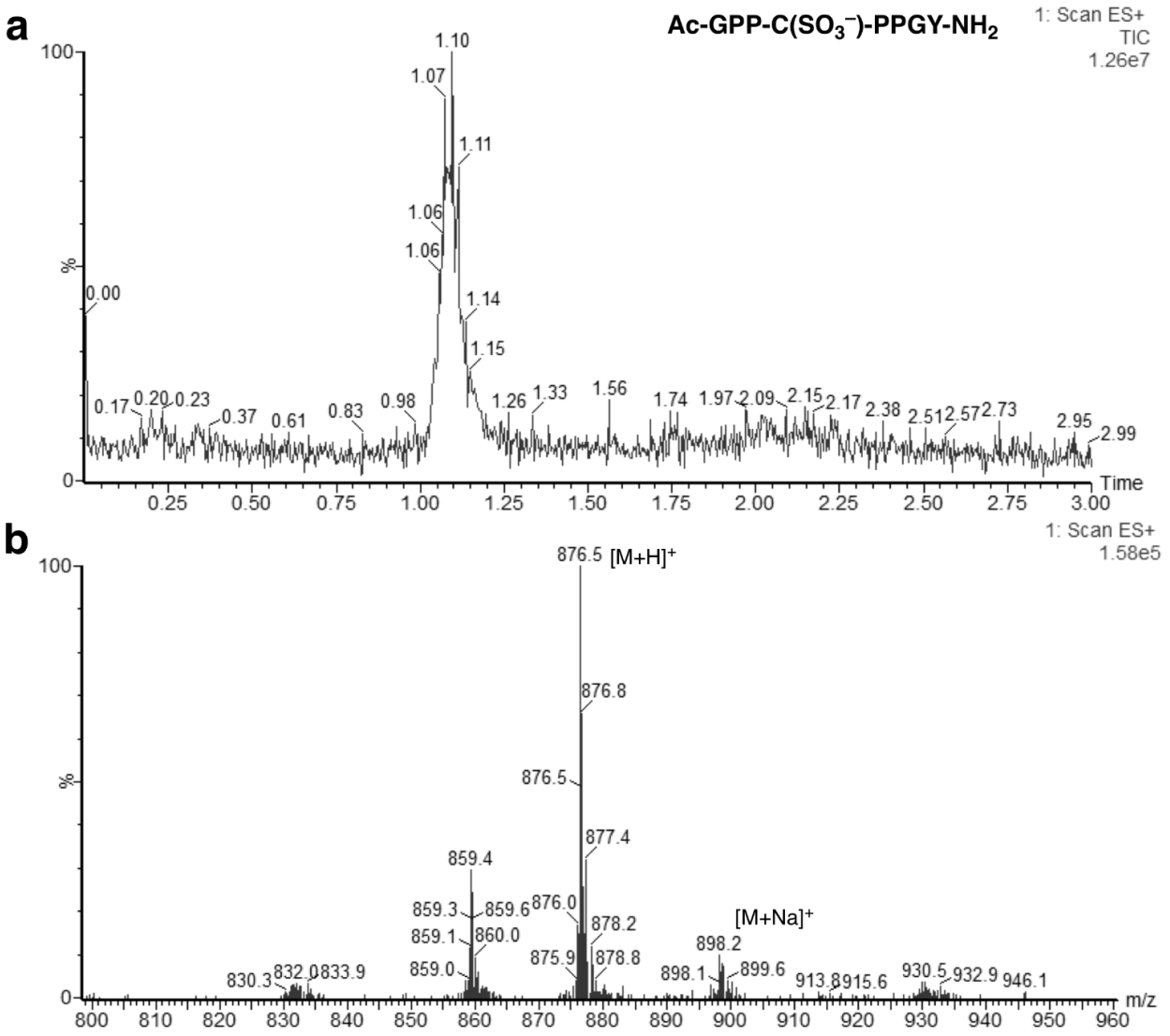


Figure S37. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-GPP-C(SO_3^-)-PPGY-NH_2. Calculated exact mass: 875.4; observed: 876.5 $[M+H]^+$, 898.2 $[M+Na]^+$.

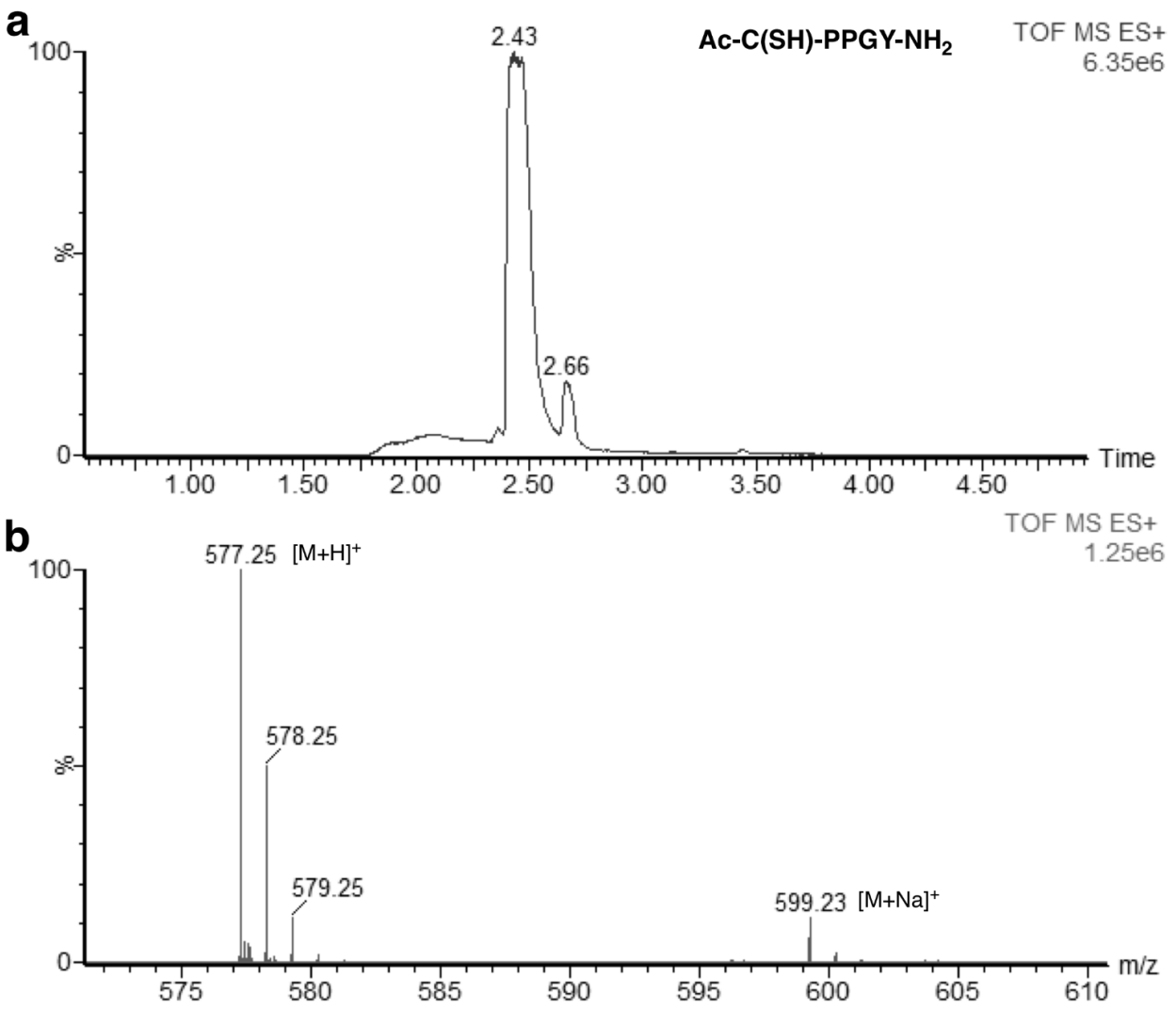


Figure S38. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-C(SH)-PPGY-NH_2. Calculated exact mass: 576.2; observed: 577.3 $[M+H]^+$, 599.2 $[M+Na]^+$.

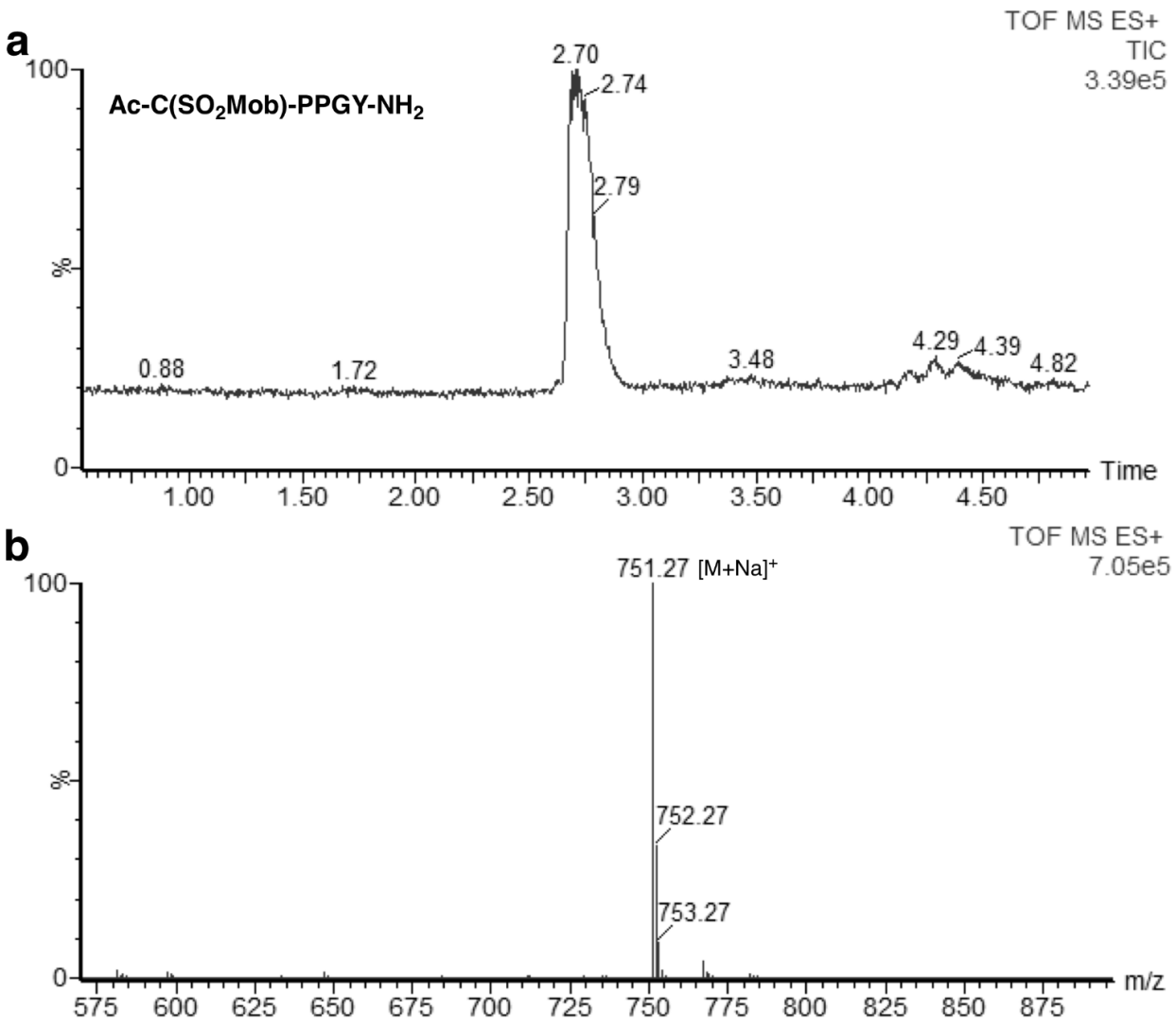


Figure S39. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-C(SO_2Mob)-PPGY-NH_2. Calculated exact mass: 728.3; observed: 751.3 $[M+Na]^+$.

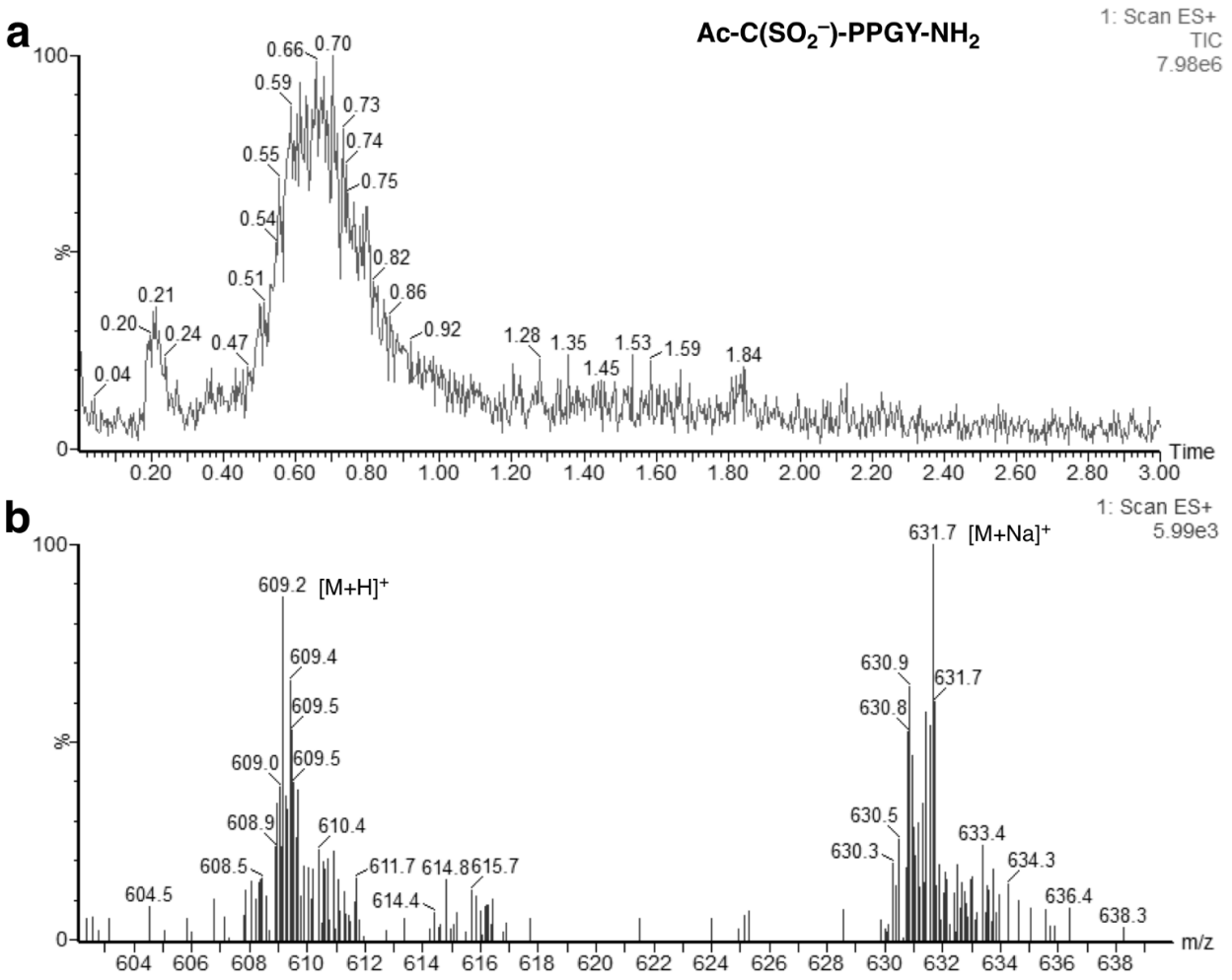


Figure S40. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-C(SO_2^-)-PPGY-NH_2. Calculated exact mass: 608.2; observed: 609.2 $[M+H]^+$, 631.7 $[M+Na]^+$.

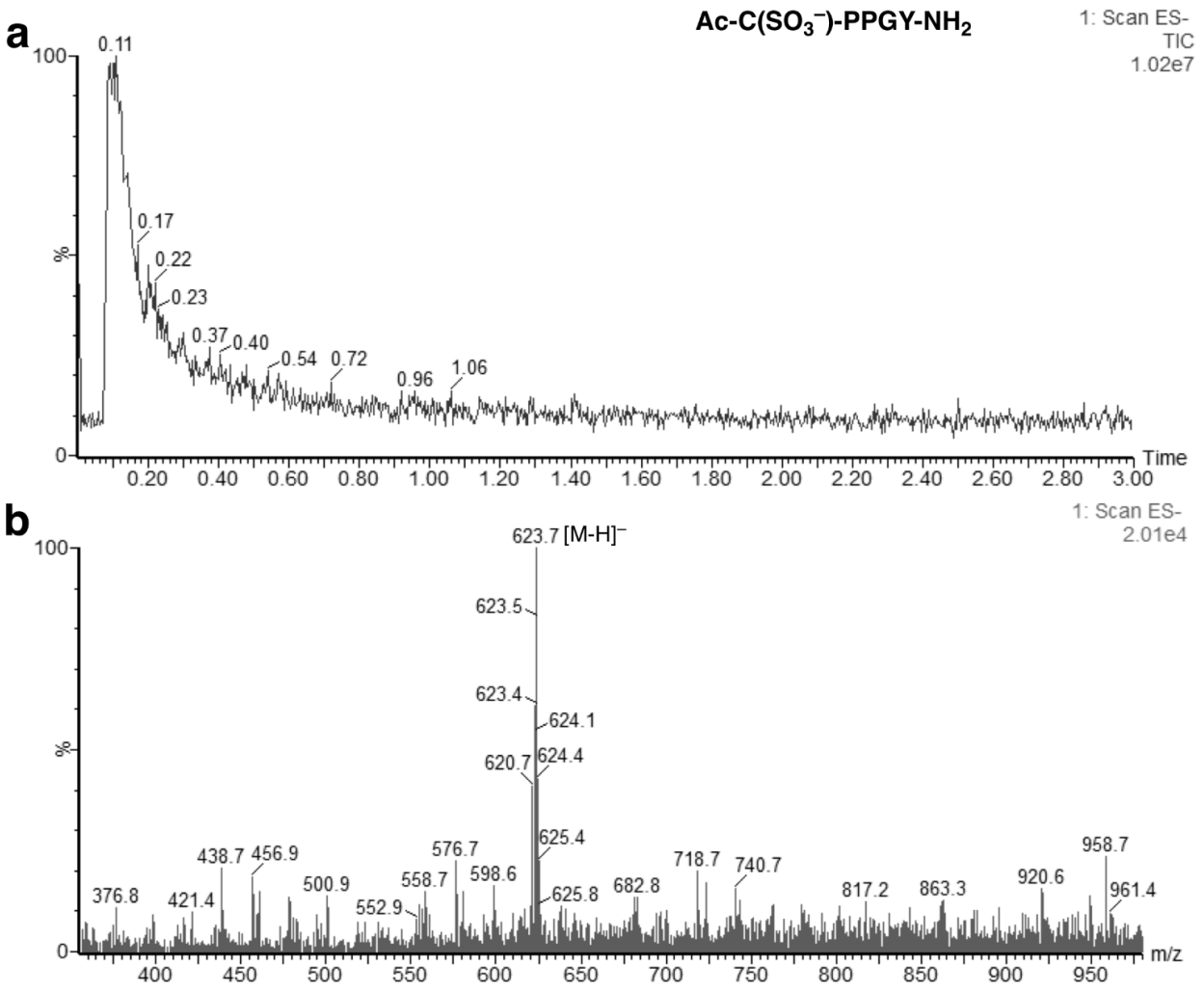


Figure S41. Negative ion mode LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-C(SO_3^-)-PPGY-NH_2. Calculated exact mass: 624.2; observed: 623.7 $[M-H]^-$.

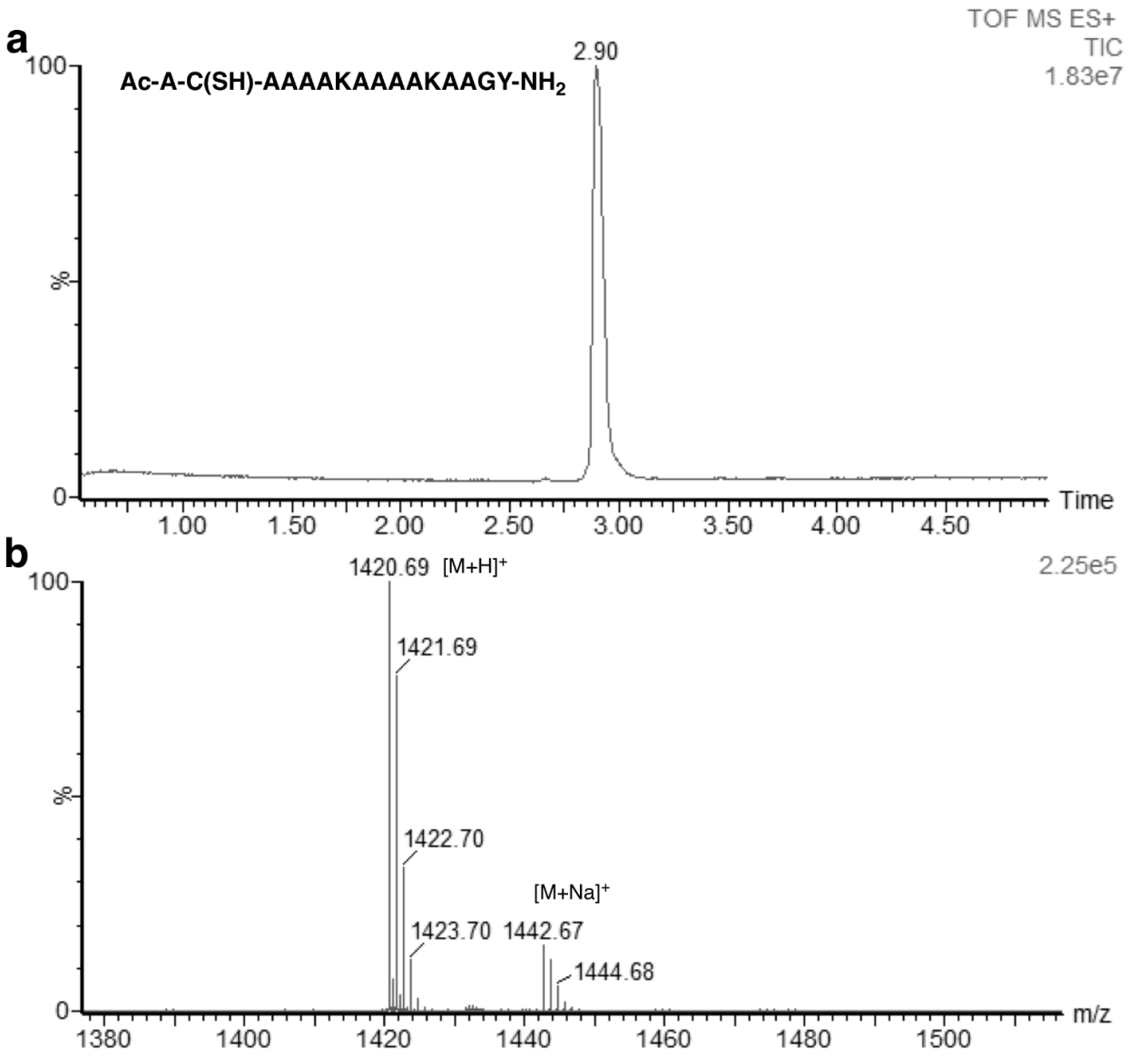


Figure S42. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-A-C(SH)-AAAAKAAAAKAAGY-NH_2. Calculated exact mass: 1419.7; observed: 1420.7 $[M+H]^+$, 1442.7 $[M+Na]^+$.

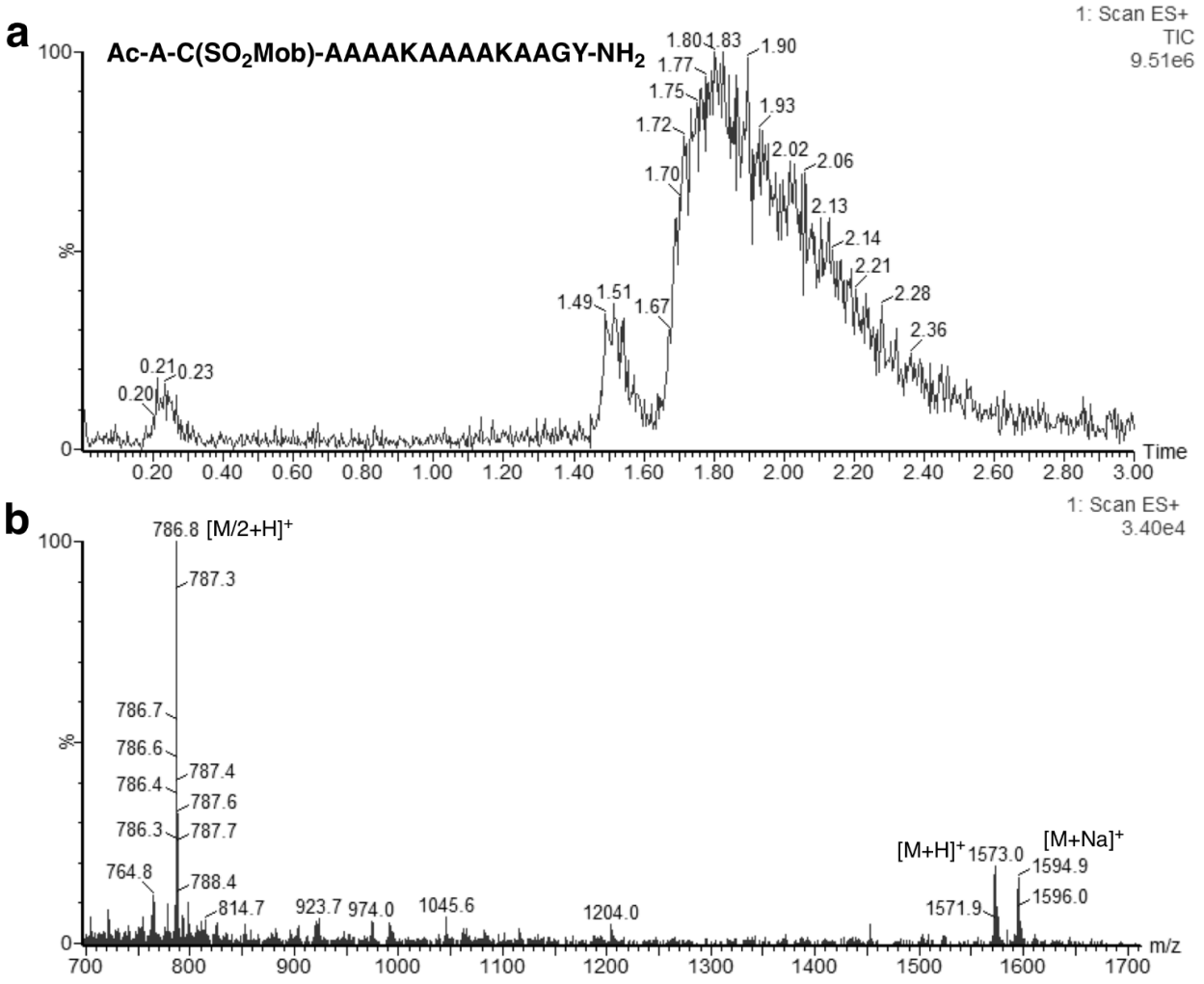


Figure S43. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-A-C(SO_2Mob)-AAAAKAAAAKAAGY-NH_2. Calculated exact mass: 1571.8; observed: 786.8 $[M/2+H]^+$, 1573.0 $[M+H]^+$, 1594.9 $[M+Na]^+$.

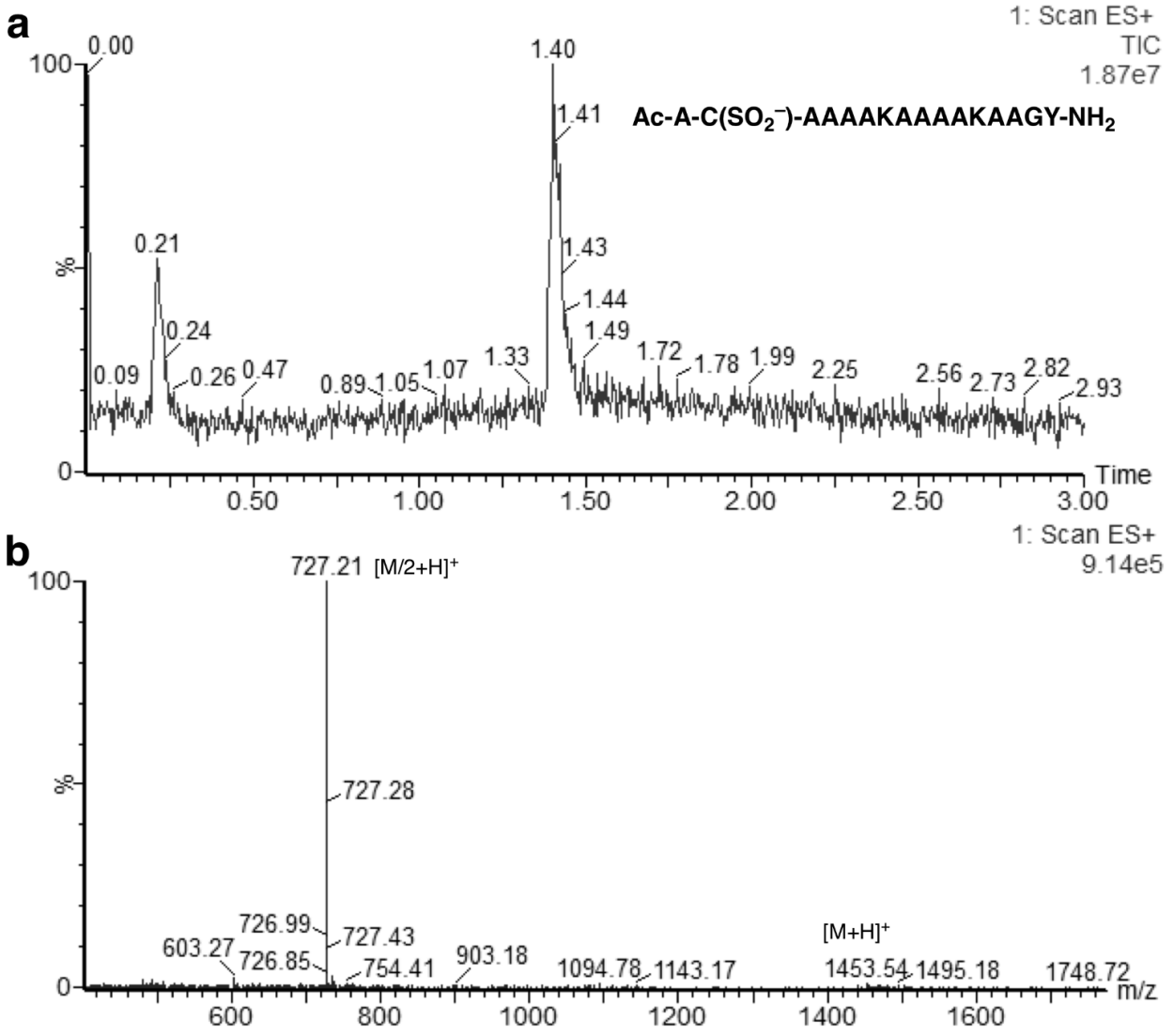


Figure S44. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-A-C(SO_2^-)-AAAAKAAAAKAAGY-NH_2. Calculated exact mass: 1451.7; observed: 727.2 $[M/2+H]^+$, 1553.5 $[M+H]^+$.

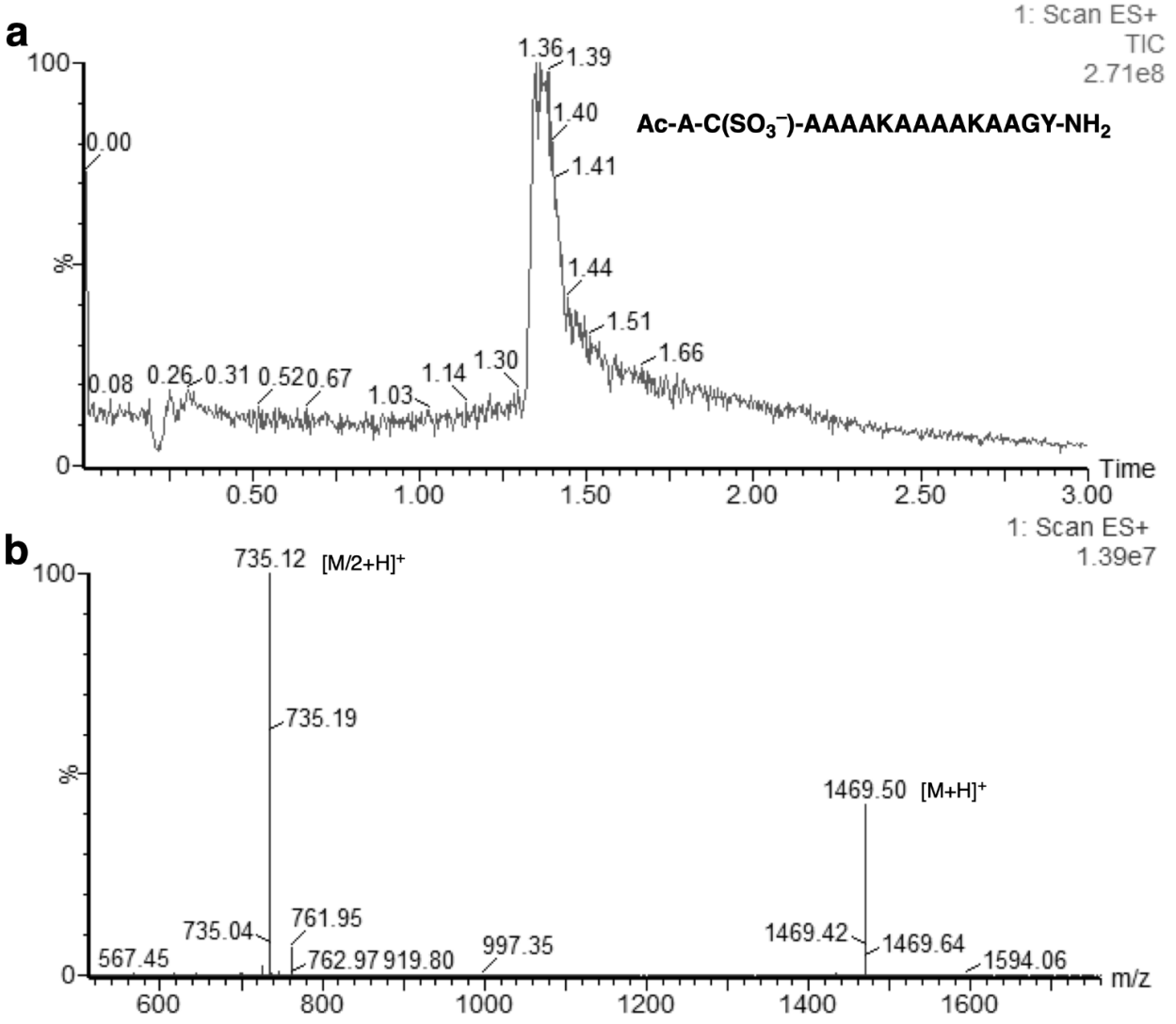


Figure S45. LC-MS (a) chromatogram and (b) mass spectrum of the peptide Ac-A-C(SO_3^-)-AAAAKAAAAKAAGY-NH_2. Calculated exact mass: 1467.7; observed: 735.1 $[M/2+H]^+$, 1469.5 $[M+H]^+$.

Comparison of structures and C–S and S–O bond lengths in cysteine, cysteine sulfinic acid, and cysteine sulfonic acid based on DFT calculations using structures with fixed ϕ and ψ (Figure 1cd)

Geometry optimization calculations of Ac-Cys(SO_2^-)-NHMe and Ac-Cys(SO_3^-)-NHMe were conducted to compare structures of cysteine oxoforms, including C–S and C–O bond lengths. Also, geometry optimization calculations of Ac-Cys(SH)-NHMe, and the structurally similar Neopentylglycine (Npg) were performed to extend the comparison. These minimal models of cysteine oxoforms and protonation states were geometry optimized with the M06-2X method and the aug-cc-pVTZ basis set in implicit H_2O (IEFPCM model), with the ϕ and ψ angles fixed at –135º and +135º, respectively. All atom positions and all other bond angles and dihedral angles were unrestrained. The restrained optimization was conducted in order to compare all molecules without the added complication of side chain-main chain hydrogen bonds or without side chain-main chain steric interactions.

Ac-Cys(SH)-NHMe

optimized M06-2X/aug-cc-pVTZ/H_2O, fixed ϕ –135º and ψ +135º

0 1

C	2.51400000	-2.35000000	-0.47600000
C	1.70500000	-1.31000000	0.25300000
O	1.97400000	-0.97500000	1.40100000
H	2.53600000	-3.25500000	0.12700000
H	3.53600000	-1.98400000	-0.56900000
H	2.12300000	-2.58000000	-1.46400000
N	0.67800000	-0.77000000	-0.43800000
C	-0.21400000	0.22200000	0.11800000
C	-1.64400000	-0.16900000	-0.24800000
O	-1.91400000	-0.51300000	-1.39300000
C	0.04900000	1.62300000	-0.43400000
S	1.71900000	2.17000000	0.05800000
H	-0.69000000	2.31500000	-0.03500000
H	0.47100000	-1.09400000	-1.37000000
H	-0.07300000	0.21600000	1.19800000
H	-0.02400000	1.60300000	-1.52000000
N	-2.55000000	-0.09200000	0.73000000
C	-3.95200000	-0.38100000	0.48900000
H	-4.07000000	-1.39500000	0.11300000
H	-2.25700000	0.18500000	1.65100000
H	-4.36400000	0.31100000	-0.24400000
H	-4.49200000	-0.27800000	1.42500000
H	1.67100000	3.35600000	-0.56300000

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12 23 1.0
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Ac-Cys(SO_2^-)-NHMe

optimized M06-2X/aug-cc-pVTZ/H_2O, fixed ϕ –135º and ψ +135º

–1 1

C	-0.90900000	3.55400000	-0.45300000
C	-0.63300000	2.25000000	0.25100000
O	-1.05500000	2.03300000	1.38000000
H	-0.59200000	4.37000000	0.19400000
H	-1.98500000	3.64200000	-0.59900000
H	-0.40900000	3.63700000	-1.41400000
N	0.09600000	1.35400000	-0.44500000
C	0.45000000	0.03600000	0.04100000
C	1.92500000	-0.19400000	-0.26900000
O	2.37800000	0.07900000	-1.37600000
C	-0.36000000	-1.06500000	-0.63500000
S	-2.10400000	-1.11500000	-0.07000000
O	-2.62300000	-2.26600000	-0.91300000
O	-1.91800000	-1.55200000	1.37200000
H	0.02700000	-2.05500000	-0.38300000
H	0.43400000	1.59500000	-1.36400000
H	0.26800000	0.01700000	1.11400000
H	-0.35600000	-0.93300000	-1.71700000
N	2.66500000	-0.71900000	0.71300000
C	4.06100000	-1.05800000	0.51500000
H	4.63100000	-0.17300000	0.23700000
H	2.23200000	-0.91400000	1.60000000
H	4.16700000	-1.80100000	-0.27500000
H	4.45500000	-1.46200000	1.44200000

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Ac-Cys(SO_3^-)-NHMe

optimized M06-2X/aug-cc-pVTZ/H_2O, fixed ϕ –135º and ψ +135º

–1 1

C	-1.09300000	3.37400000	-0.50600000
C	-0.51600000	2.22600000	0.27900000
O	-0.70900000	2.10500000	1.48200000
H	-1.07400000	4.27200000	0.10500000
H	-2.13200000	3.13100000	-0.72800000
H	-0.56900000	3.55000000	-1.44200000
N	0.22000000	1.34800000	-0.43800000
C	0.65200000	0.06800000	0.07300000
C	2.12200000	-0.13000000	-0.29000000
O	2.51600000	0.10200000	-1.42800000
C	-0.12100000	-1.10200000	-0.53800000
S	-1.83300000	-1.22600000	-0.00400000
O	-2.32500000	-2.45500000	-0.65000000
O	-1.78300000	-1.33000000	1.46300000
H	0.33800000	-2.04700000	-0.24600000
H	0.31300000	1.49100000	-1.43100000
H	0.50900000	0.08300000	1.15200000
H	-0.12700000	-1.03300000	-1.62500000
N	2.91600000	-0.59300000	0.68000000
C	4.31600000	-0.88900000	0.43900000
H	4.85100000	0.01200000	0.14100000
H	2.53200000	-0.74200000	1.59800000
H	4.41700000	-1.62900000	-0.35300000
H	4.75000000	-1.27800000	1.35400000
O	-2.52200000	-0.01700000	-0.47900000

1 2 1.0 4 1.0 5 1.0 6 1.0
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Ac-Npg-NHMe

optimized M06-2X/aug-cc-pVTZ/H_2O, fixed ϕ –135º and ψ +135º

0 1

C	-1.10700000	3.44900000	-0.47700000
C	-0.70300000	2.20300000	0.26700000
O	-1.05900000	2.00600000	1.42500000
H	-0.88500000	4.31500000	0.14400000
H	-2.18500000	3.41400000	-0.63200000
H	-0.61200000	3.55200000	-1.43900000
N	0.04100000	1.32100000	-0.42500000
C	0.48600000	0.04500000	0.09900000
C	1.95700000	-0.10400000	-0.27600000
O	2.33700000	0.14800000	-1.41500000
C	-0.25000000	-1.16800000	-0.49000000
H	0.33900000	-2.05000000	-0.21900000
H	0.31900000	1.53700000	-1.37000000
H	0.36900000	0.08200000	1.18100000
H	-0.20600000	-1.08500000	-1.58000000
N	2.77700000	-0.54100000	0.68600000
C	4.18300000	-0.79300000	0.42900000
H	4.68000000	0.12000000	0.10600000
H	2.40500000	-0.71900000	1.60200000
H	4.30100000	-1.54600000	-0.35000000
H	4.64400000	-1.14800000	1.34400000
C	-2.09300000	-2.78800000	-0.65500000
H	-3.12300000	-3.03600000	-0.39400000
H	-2.01400000	-2.76900000	-1.74400000
H	-1.44500000	-3.58200000	-0.28000000
C	-1.80700000	-1.50900000	1.46600000
H	-2.80900000	-1.83200000	1.75500000
H	-1.09100000	-2.22800000	1.87200000
H	-1.62400000	-0.53600000	1.92300000
C	-1.70100000	-1.43300000	-0.05700000
C	-2.67100000	-0.37400000	-0.58500000
H	-2.53900000	0.58100000	-0.08000000
H	-2.54100000	-0.22400000	-1.65900000
H	-3.69900000	-0.69900000	-0.41000000

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31 32 1.0 33 1.0 34 1.0
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Calculations on Ac-Cys(SO_3^-)-NHMe (structures for Figure 18)

To gain more insight into the conformational preferences of cysteine sulfonate, as well as the interactions between SO_i•••HN_i, SO_i•••HN_{i+1}, SO_i•••CO_{i-1} that occur in peptides and proteins containing cysteine sulfonic acid, DFT calculations were performed on simplified models of the peptide Ac-Cys(SO_3^-)-NHMe in six different regions of Ramachandran space (α_R, PPII, β, α_L, cluster I, $PPII_R$, inverse γ, and classic γ) and in three different rotameric states (g^-, g^+, and t). The geometry optimization calculations were performed using iterative methods, with the final calculations performed using the M06-2X DFT functional and the 6-311++G(2d,2p) basis set with implicit H_2O (IEFPCM model). The optimized structures were then checked for imaginary frequencies, and none were found, indicating that they represent local minima. The energies were calculated using the MP2 method and the 6-311++G(2d,2p) basis set with implicit H_2O (IEFPCM model), and the relative energy for each peptide was determined with respect to the minimum energy model, which was defined as $E_{rel} = 0.0$ kcal mol^{-1}.

The coordinates of the optimized structures are given below.

Figure 18a

Ac-Cys(SO_3^-)-NHMe, α_R g^-

optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	1.16590200	3.29788900	-0.43045000
C	1.24891800	1.93960900	0.21563600
O	2.02604700	1.69744000	1.12929200
H	2.16863200	3.61421200	-0.70883100
H	0.78210300	4.00410200	0.30452600
H	0.52294500	3.30640700	-1.30646700
N	0.42159100	0.98510700	-0.28206400
C	0.28517400	-0.27701700	0.41873900
C	1.54513500	-1.14355400	0.34907900
O	1.74753000	-1.99710600	1.20511100
C	-0.86220500	-1.09903000	-0.15913400
S	-2.45157500	-0.26533300	-0.07107800
O	-3.43277100	-1.27457700	-0.46972200
O	-2.59249000	0.18243500	1.31609600
H	-0.96287000	-2.02261100	0.40559300
H	-0.35874000	1.26872900	-0.86275700
H	0.10242700	-0.09953200	1.47923200
H	-0.69530600	-1.33431300	-1.20994300
N	2.33716200	-0.96646300	-0.71367200
C	3.54020600	-1.75479900	-0.89845300
H	3.29665900	-2.81545100	-0.91566600
H	2.12992500	-0.20832800	-1.34179700
H	4.24888900	-1.57544600	-0.09057200
H	3.99698100	-1.47721200	-1.84278400
O	-2.35537800	0.85126700	-1.02773200

1 2 1.0 4 1.0 5 1.0 6 1.0
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7 8 1.0 16 1.0
8 9 1.0 11 1.0 17 1.0
9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
12 13 2.0 14 2.0 25 2.0
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20 21 1.0 23 1.0 24 1.0
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Figure 18b
Ac-Cys(SO_3^-)-NHMe, α_R g^+
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1
C -2.79998700 -2.37406600 -0.79476500
C -2.32348400 -1.28282200 0.12965400
O -3.07908500 -0.72540300 0.91634100
H -3.68021800 -2.02119000 -1.32741500
H -3.09437200 -3.23041800 -0.18960300
H -2.04022700 -2.68419400 -1.50718000
N -1.01272300 -0.95791800 0.03780300
C -0.39958100 -0.01348200 0.94620000
C -0.50375600 1.45477500 0.51302100
O -0.08399100 2.33279700 1.25897600
C 1.04883600 -0.38595500 1.25405000
S 2.10932600 -0.51805400 -0.19002500
O 3.43719800 -0.82768400 0.34014500
O 1.54354300 -1.61667400 -0.99484800
H 1.09679900 -1.35019700 1.75554000
H -0.39574200 -1.46852500 -0.58278200
H -0.95203200 -0.05426600 1.88624000
H 1.48917700 0.37687200 1.89068100
N -1.10572000 1.70993800 -0.65213300
C -1.20369800 3.06413700 -1.15987400
H -0.21328400 3.48983500 -1.32116000
H -1.34148300 0.93424100 -1.24675400
H -1.73805000 3.69261400 -0.45003800
H -1.74611300 3.04670000 -2.09958000
O 2.03051500 0.77668100 -0.87023400

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9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
12 13 2.0 14 2.0 25 2.0
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20 21 1.0 23 1.0 24 1.0
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Figure 18c
Ac-Cys(SO_3^-)-NHMe, α_R *t*
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1
C -3.91175200 -1.66587600 -0.52730300
C -2.76426200 -0.97916400 0.16625300
O -2.91025400 -0.35544600 1.20842600
H -4.68456900 -0.92624300 -0.72707000
H -4.32621500 -2.40939200 0.15110000
H -3.62022700 -2.14725200 -1.45664600
N -1.55074900 -1.07548300 -0.42759500
C -0.36227300 -0.51362200 0.19563500
C -0.48454200 1.00970400 0.35596800
O -0.16023000 1.56869200 1.39243100
C 0.83483300 -0.93215100 -0.65433300
S 2.44082000 -0.43617500 -0.01983000
O 3.39217300 -1.16698400 -0.86289800
O 2.51628000 1.01540600 -0.19640300
H 0.76710600 -0.52540800 -1.66303600
H -1.44989800 -1.64974900 -1.24833800
H -0.25044100 -0.90796200 1.20481100
H 0.86768800 -2.01930500 -0.71299300
N -0.94294600 1.67184600 -0.71772200
C -1.09086900 3.11398700 -0.70150900
H -0.12862600 3.58933300 -0.51806000
H -1.28076700 1.14766400 -1.50686600
H -1.78401200 3.42329600 0.08017300
H -1.47065000 3.43754100 -1.66524300
O 2.46660000 -0.86236000 1.38199500

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5
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7 8 1.0 16 1.0
8 9 1.0 11 1.0 17 1.0
9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
12 13 2.0 14 2.0 25 2.0
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19 20 1.0 22 1.0
20 21 1.0 23 1.0 24 1.0
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Figure 18d
Ac-Cys(SO_3^-)-NHMe, PPII *g*$^-$
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	0.87229300	3.52157600	-0.19963600
C	1.14375500	2.08774900	0.17663100
O	2.13803700	1.76048200	0.81727000
H	1.76064200	3.93275700	-0.67376900
H	0.68621200	4.08619700	0.71291100
H	0.02003200	3.62599100	-0.86579100
N	0.23324500	1.17954300	-0.22653800
C	0.34311300	-0.19957600	0.19125500
C	1.65837100	-0.80974900	-0.30941100
O	2.06798900	-0.60939500	-1.44364800
C	-0.79303100	-1.03342000	-0.39206600
S	-2.42527400	-0.43217100	0.06245200
O	-3.35386500	-1.46612900	-0.39451800
O	-2.39659100	-0.26329900	1.51708900
H	-0.72754000	-2.05426000	-0.02205000
H	-0.64883100	1.47829200	-0.62180600
H	0.30844800	-0.25967200	1.28150200
H	-0.75408800	-1.03950200	-1.48036600
N	2.26663600	-1.64139300	0.54904400
C	3.49581600	-2.32291800	0.18842500
H	4.29796400	-1.60693600	0.01155400
H	1.93758500	-1.69229500	1.49758300
H	3.34707400	-2.90754000	-0.71719700
H	3.77809800	-2.98514400	1.00034000
O	-2.58335400	0.84181900	-0.66005100

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5
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7 8 1.0 16 1.0
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9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
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19 20 1.0 22 1.0
20 21 1.0 23 1.0 24 1.0
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Figure 18e
Ac-Cys(SO_3^-)-NHMe, PPII g^+
optimized M06-2X/6-311++G(2d,2p)p/H_2O

-1 1

C	-3.29883200	-1.93783200	-0.63913300
C	-2.60691500	-0.86434800	0.16187600
O	-3.23527000	0.02560500	0.72558900
H	-3.79800600	-1.46571000	-1.48400700
H	-4.06063500	-2.40233500	-0.01655900
H	-2.61364100	-2.69760700	-1.00556100
N	-1.26192200	-0.95275300	0.23719500
C	-0.49129900	0.10692900	0.83575000
C	-0.44190800	1.34191300	-0.08618100
O	-0.84522300	1.31325500	-1.23799000
C	0.89171200	-0.39591400	1.25274500
S	1.96770100	-0.89382300	-0.09923400
O	3.12752000	-1.50261900	0.55437600
O	1.18632700	-1.85561300	-0.89534000
H	0.78240800	-1.26820700	1.89401600
H	-0.75816300	-1.58264900	-0.37306500
H	-1.01080200	0.41734300	1.74359200
H	1.44008900	0.36933300	1.79727400
N	0.04603200	2.45471700	0.48515100
C	0.22840000	3.67287300	-0.28130800
H	-0.71853700	3.99717800	-0.70876500
H	0.36972700	2.42371000	1.43644300
H	0.93979100	3.51435700	-1.09147600
H	0.60524400	4.44666400	0.37967900
O	2.28709500	0.33107400	-0.83447800

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9 10 2.0 19 1.5
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Figure 18f
Ac-Cys(SO_3^-)-NHMe, PPII *t*
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	-4.23476400	-1.15332600	-0.29631400
C	-2.97137400	-0.57052200	0.28190200
O	-2.99028800	0.27738800	1.16524400
H	-4.76023800	-0.36404100	-0.83214400
H	-4.87044700	-1.48549700	0.52130800
H	-4.04696700	-1.98210500	-0.97357500
N	-1.80620700	-1.03976200	-0.22091000
C	-0.54610700	-0.44512900	0.16817400
C	-0.46455800	1.01174600	-0.31658100
O	-0.97419200	1.36188700	-1.37221600
C	0.58498400	-1.30139300	-0.39599300
S	2.22800500	-0.71168500	0.04617400
O	3.10540500	-1.86831900	-0.13499300
O	2.52071500	0.39352400	-0.86909900
H	0.55266200	-1.33812500	-1.48445200
H	-1.83423900	-1.61493000	-1.04661200
H	-0.48294900	-0.45163200	1.25518100
H	0.50256100	-2.31062200	0.00179600
N	0.19772300	1.84325300	0.50327700
C	0.56141000	3.17165600	0.04807400
H	-0.33205300	3.72248800	-0.23556400
H	0.78749800	1.40353600	1.19807200
H	1.22992900	3.11975500	-0.81260200
H	1.05772200	3.69532300	0.85947300
O	2.11714800	-0.27820700	1.44833900

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9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
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Figure 18g
Ac-Cys(SO_3^-)-NHMe, βg^-
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	-0.98736300	3.46564800	-0.46629500
C	-0.44246800	2.28316300	0.29356100
O	-0.58040400	2.17611100	1.50590800
H	-0.90534700	4.35555900	0.15101600
H	-2.04344000	3.27721900	-0.66145500
H	-0.48202800	3.62357300	-1.41601700
N	0.18460300	1.35277600	-0.45877100
C	0.61993800	0.07584600	0.05205200
C	2.09961800	-0.11672600	-0.27989300
O	2.54914700	0.23954500	-1.36246900
C	-0.14687200	-1.09181700	-0.57362300
S	-1.84871700	-1.23366300	-0.01191900
O	-2.34418600	-2.44580000	-0.67325000
O	-1.76277600	-1.36542100	1.44670200
H	0.32160600	-2.03784800	-0.30540600
H	0.27313200	1.50397800	-1.45037500
H	0.46124400	0.08357100	1.12871600
H	-0.16885600	-1.00437300	-1.65924700
N	2.83746600	-0.73442600	0.65110000
C	4.23301000	-1.06020900	0.41716200
H	4.79629000	-0.15974400	0.17992400
H	2.41372500	-0.98276200	1.52841700
H	4.32918100	-1.75940600	-0.41206600
H	4.63919200	-1.51125900	1.31646600
O	-2.54489100	-0.01865600	-0.44355800

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5
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8 9 1.0 11 1.0 17 1.0
9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
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19 20 1.0 22 1.0
20 21 1.0 23 1.0 24 1.0
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Figure 18h
Ac-Cys(SO_3^-)-NHMe, βg^+
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	3.79394700	-0.52482100	-0.86348600
C	2.70791900	-0.64956700	0.17475800
O	2.96201800	-0.66226200	1.37649300
H	4.54320700	-1.29182300	-0.67926600
H	4.27148700	0.44663200	-0.74429000
H	3.41872400	-0.61834100	-1.87900900
N	1.44959000	-0.74961200	-0.29252600
C	0.30941600	-0.76027900	0.58949800
C	-0.85614700	-1.43697700	-0.13661600
O	-0.82058100	-1.65932200	-1.33890500
C	-0.03713000	0.63835000	1.12016900
S	-0.72740900	1.77069100	-0.09322400
O	-0.76011000	3.06531500	0.59494800
O	0.18384100	1.74967800	-1.24293900
H	0.87083200	1.09852400	1.50466500
H	1.25480800	-0.62039000	-1.27261900
H	0.57086000	-1.36858900	1.45626500
H	-0.76758000	0.58476500	1.92548700
N	-1.89413700	-1.78196700	0.63802800
C	-3.12367900	-2.27799900	0.04873200
H	-2.93507100	-3.20199800	-0.49405500
H	-1.89067500	-1.51908000	1.60878100
H	-3.53714000	-1.54420000	-0.64276200
H	-3.83827900	-2.47032100	0.84231200
O	-2.06226200	1.25191300	-0.40844400

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5
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7 8 1.0 16 1.0
8 9 1.0 11 1.0 17 1.0
9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
12 13 2.0 14 2.0 25 2.0
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19 20 1.0 22 1.0
20 21 1.0 23 1.0 24 1.0
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Figure 18i
Ac-Cys(SO_3^-)-NHMe, βt
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1
C -4.39496200 -0.05591000 -0.33970300
C -3.02469200 -0.34433100 0.21813100
O -2.83388900 -1.23937400 1.03532900
H -5.09017900 0.06000300 0.48875700
H -4.71297200 -0.91584700 -0.92740700
H -4.41851600 0.83329100 -0.96389700
N -2.02079800 0.43354700 -0.23399400
C -0.64978900 0.24039200 0.18490000
C 0.10128900 1.54239800 -0.09068700
O -0.22410800 2.26147400 -1.02989800
C -0.03237100 -0.94899400 -0.56366400
S 1.67764200 -1.27994800 -0.11806300
O 1.91649400 -2.67542100 -0.48789300
O 2.48445100 -0.32619700 -0.88455100
H -0.05288000 -0.78505600 -1.63949200
H -2.18365400 1.14260200 -0.93260900
H -0.63560200 0.02174900 1.25078600
H -0.60263300 -1.84187300 -0.31775600
N 1.10079200 1.82117400 0.75505100
C 2.04549000 2.87770700 0.44256600
H 1.51325700 3.81028500 0.27495200
H 1.42350800 1.04958200 1.32666100
H 2.61883700 2.63108700 -0.45229800
H 2.72244700 3.00047600 1.28221000
O 1.75034700 -1.04270200 1.33481800

1 2 1.0 4 1.0 5 1.0 6 1.0
2 3 2.0 7 1.5
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7 8 1.0 16 1.0
8 9 1.0 11 1.0 17 1.0
9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
12 13 2.0 14 2.0 25 2.0
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19 20 1.0 22 1.0
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Figure 18j
Ac-Cys(SO_3^-)-NHMe, α_L g^-
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1
C -0.01476300 3.16901700 0.09203300
C 0.47716600 1.78494600 -0.23001600
O 0.94323700 1.47751100 -1.31629500
H -1.09666900 3.16825600 -0.04388100
H 0.43505000 3.88294600 -0.59053000
H 0.20376600 3.44418100 1.12184000
N 0.37792400 0.87462800 0.78306200
C 0.44709800 -0.54814600 0.48877900
C 1.84043300 -0.97310500 0.01499200
O 1.98985900 -1.92645600 -0.73940000
C -0.62430300 -1.03402500 -0.48201200
S -2.26533400 -0.50918200 0.02995100
O -3.19502600 -1.40451400 -0.66597600
O -2.28627300 -0.66615000 1.49165100
H -0.63323500 -2.11960100 -0.50653000
H -0.23191900 1.12333600 1.54747000
H 0.28900000 -1.05617300 1.44067500
H -0.46466100 -0.65084000 -1.48623600
N 2.86752800 -0.29303300 0.54190400
C 4.23691700 -0.59876700 0.17717600
H 4.41165800 -0.40625900 -0.88141200
H 2.66328100 0.53264600 1.07900000
H 4.45406600 -1.64582500 0.37843600
H 4.90130000 0.02332600 0.76846400
O -2.39926500 0.89213900 -0.38835300

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7 8 1.0 16 1.0
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9 10 2.0 19 1.5
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11 12 1.0 15 1.0 18 1.0
12 13 2.0 14 2.0 25 2.0
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19 20 1.0 22 1.0
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Figure 18k
Ac-Cys(SO_3^-)-NHMe, cluster I g^+
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	3.60179400	1.22459600	-0.97320900
C	2.80135700	0.47208500	0.06060400
O	3.33626300	-0.01185300	1.05243900
H	4.34027400	0.54548400	-1.39581600
H	4.13497000	2.03261500	-0.47616900
H	2.98758300	1.63150800	-1.77204500
N	1.47757600	0.37591600	-0.18182300
C	0.55975100	-0.29612700	0.71085700
C	0.16332600	-1.66355100	0.12670800
O	1.04708300	-2.42344400	-0.25367900
C	-0.54356000	0.64828400	1.18847400
S	-1.68143000	1.27865200	-0.06899900
O	-2.06765100	2.61186700	0.38739500
O	-0.93247100	1.28258600	-1.33376900
H	-0.07077300	1.52757100	1.61894900
H	1.07094900	0.82129300	-0.99103800
H	1.14600900	-0.55543500	1.59424400
H	-1.16269400	0.18163800	1.95209000
N	-1.13218100	-2.00322000	0.12481700
C	-1.54088700	-3.29220800	-0.40405600
H	-1.04099600	-4.09299500	0.13660400
H	-1.84017700	-1.28350600	0.22045000
H	-1.28981000	-3.38259000	-1.46104500
H	-2.61467500	-3.39261800	-0.27921700
O	-2.81150300	0.33350000	-0.08991600

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Figure 18l
Ac-Cys(SO_3^-)-NHMe, $PPII_R$ *t*
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	-3.78535700	-1.77628800	0.11461400
C	-2.49249700	-1.09372900	-0.25090700
O	-2.24937600	-0.73125900	-1.39469600
H	-3.98846800	-2.55567100	-0.61579800
H	-4.58588500	-1.03969200	0.05465000
H	-3.76982800	-2.20379100	1.11364100
N	-1.60382800	-0.91385100	0.75400200
C	-0.42102000	-0.10423000	0.56304100
C	-0.81637300	1.36606600	0.30064500
O	-1.95749600	1.76552900	0.49138200
C	0.51076000	-0.70354300	-0.50507600
S	2.23274600	-0.73612700	-0.00276400
O	2.93940600	-1.39687200	-1.10059600
O	2.62781000	0.67595700	0.16584300
H	0.46394400	-0.16991200	-1.45025800
H	-1.90443400	-1.09843700	1.69547300
H	0.10849600	-0.11054600	1.51778700
H	0.24601800	-1.74253800	-0.68195600
N	0.18111200	2.16330200	-0.10182200
C	-0.03709200	3.58498700	-0.28751800
H	-0.34748500	4.05991000	0.64333100
H	1.12666800	1.79290100	-0.11285100
H	-0.81085200	3.75512100	-1.03400900
H	0.88970400	4.03628700	-0.62824400
O	2.27174000	-1.47977300	1.25911800

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9 10 2.0 19 1.5
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Figure 18m
Ac-Cys(SO_3^-)-NHMe, γ' g^-
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	0.58071800	3.27677100	-0.68076400
C	0.90973800	1.98034700	0.01009100
O	1.65064200	1.94453700	0.99188600
H	1.50460400	3.82045600	-0.86315900
H	-0.03507300	3.87358000	-0.00887500
H	0.04929700	3.13049500	-1.61712100
N	0.34948100	0.86789500	-0.50752700
C	0.36773700	-0.40282700	0.20949900
C	1.65116100	-1.19303200	-0.11102400
O	1.62900100	-2.24770100	-0.73430800
C	-0.84854500	-1.24179900	-0.14003400
S	-2.40240500	-0.37518500	0.10359000
O	-3.43237000	-1.41307900	0.03140400
O	-2.30848100	0.26904300	1.41668600
H	-0.87574000	-2.12599700	0.49115500
H	-0.39766500	0.98888100	-1.17882600
H	0.36413800	-0.17959100	1.27768800
H	-0.82881300	-1.56000300	-1.18029500
N	2.77904200	-0.63564300	0.34639900
C	4.07339400	-1.22783700	0.06909900
H	4.27509100	-1.24178100	-1.00178600
H	2.70797300	0.26627200	0.79969100
H	4.10793600	-2.25119600	0.43859200
H	4.83838600	-0.64250400	0.56918600
O	-2.48585800	0.59080500	-1.00529300

1 2 1.0 4 1.0 5 1.0 6 1.0
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11 12 1.0 15 1.0 18 1.0
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Figure 18n
Ac-Cys(SO_3^-)-NHMe, γg^-
optimized M06-2X/6-311++G(2d,2p)/H_2O

-1 1

C	-0.30979000	3.24237900	0.49913900
C	0.29451100	1.94296500	0.04452800
O	0.72861600	1.79332300	-1.09525400
H	-1.36776400	3.21148200	0.23690500
H	0.16428500	4.06462500	-0.02823500
H	-0.22143300	3.38705100	1.57336900
N	0.32923200	0.95361400	0.96632800
C	0.48400500	-0.46615500	0.66460800
C	1.92596300	-0.92422100	0.41490700
O	2.31911800	-1.98227900	0.89789400
C	-0.40467300	-0.95819300	-0.47873000
S	-2.15288900	-0.66146000	-0.17239900
O	-2.85187600	-1.52774200	-1.12712800
O	-2.37306200	-1.04085200	1.22850600
H	-0.29176400	-2.03657800	-0.57357000
H	-0.11533000	1.15364900	1.84685500
H	0.17906400	-0.99306200	1.56425500
H	-0.16296200	-0.47935100	-1.42392000
N	2.68614300	-0.14912000	-0.36481300
C	4.04343600	-0.53469900	-0.70033000
H	4.05897200	-1.50203200	-1.20136000
H	2.24942400	0.64833000	-0.81046500
H	4.65351000	-0.60384700	0.19901900
H	4.46505800	0.21741800	-1.35944800
O	-2.38194100	0.76652100	-0.42156400

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Computational analysis of NH•••OS, OH•••OS, and Mg^{2+}•••OS interactions for methyl sulfonate and methyl sulfinate (structures from Figure 19)

In order to gain a deeper understanding of the impact that interactions involving cysteine oxoforms have on the structure of peptides and proteins, as well as the differences in interactions between cysteine sulfonate and cysteine sulfinate, a series of geometry optimization calculations were conducted on minimal models of cysteine oxoforms such as methyl sulfonate ($MeSO_3^-$) and methyl sulfinate ($MeSO_2^-$). These small-molecule structures were generated as isolated molecules, as well as in complexed bound to H_2O, methyl acetamide (AcNHMe), or Mg^{2+}. Iterative geometry optimization methods were used to generate these structures, and the final optimizations were performed using the M06-2X DFT functional and the aug-cc-pVTZ basis set in implicit water (IEFPCM). All final geometry-optimized structures were then subjected to frequency calculations using same combination of method, basis set, and solvation. The results of these calculations indicated zero negative (imaginary) frequencies, indicating that all of the optimized structures were energy minima. To further evaluate the interactions between these compounds and other molecules, the interaction energies of these complexes were determined via component energy analysis. This technique involves calculating the energy of the complex and then subtracting the energies of the individual, geometry-optimized molecules to determine the interaction energy in kcal mol^{-1}. All interaction energy calculations were conducted using the MP2 method and the aug-cc-pVQZ basis set in implicit water (IEFPCM). This larger basis set was chosen for energy calculations than that used for geometry optimization in order to minimize the basis set superposition error (BSSE). Counterpoise calculations revealed that the basis set superposition error was less than 10% of the total interaction energy for all complexes, including those in an aqueous environment. The key parameters and the coordinates of the optimized structures are given below.

interaction complex	*E*, hartrees	complex *E*, kcal mol^{-1}	N–H Å	O•••HN Å	O•••HO Å	O•••M Å
AcNHMe•••$^{-}$O$_3$SMe	-911.363723	–6.70	1.017	1.839		
HOH•••$^{-}$O$_3$SMe	-739.568763	–6.04			1.785	
Mg^{2+}•••$^{-}$O$_3$SMe	-862.698681	–24.4				2.049

Table S10. Key parameters of geometry-optimized structures of complexes representing NH•••OS, OH•••OS, and Mg^{2+}•••OS interactions with methyl sulfonate in H_2O.

interaction complex	*E*, hartrees	complex *E*, kcal mol^{-1}	N–H Å	O•••HN Å	O•••HO Å	O•••M Å
AcNHMe•••$^{-}$O$_2$SMe	-836.168744	–8.32	1.027	1.775		
HOH•••$^{-}$O$_2$SMe	-664.373508	–7.49			1.689	
Mg^{2+}•••$^{-}$O$_2$SMe	-787.518107	–35.0				2.017

Table S11. Key parameters of geometry-optimized structures of complex representing NH•••$^{-}$OS, OH•••$^{-}$OS, and Mg^{2+}•••$^{-}$OS interactions with methyl sulfinate in H_2O.

molecule	*E*, hartrees
AcNHMe	-248.152415
H_2O	-76.358503
$MeSO_2^-$	-588.003073
$MeSO_3^-$	-663.200639

Table S12. The energies in hartrees of geometry optimized individual components of structural complex presented in the tables above.

AcNHMe•••$^{-}$$O_3$SMe

optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1

C	-2.92000000	0.45400000	0.04000000
O	-4.14600000	0.33600000	0.06600000
C	-2.25500000	1.80700000	0.08800000
H	-1.17000000	1.73300000	0.06600000
H	-2.59700000	2.39500000	-0.76200000
H	-2.57000000	2.31900000	0.99500000
N	-2.09800000	-0.60000000	-0.03300000
C	-2.60700000	-1.95300000	-0.09200000
H	-1.76500000	-2.63700000	-0.15000000
H	-3.19500000	-2.18700000	0.79500000
H	-3.24200000	-2.09300000	-0.96700000
H	-1.09700000	-0.44000000	-0.05500000
O	0.73900000	-0.14800000	-0.09500000
O	2.83500000	-0.51400000	-1.31100000
O	2.54300000	1.50300000	0.05900000
S	2.19900000	0.08500000	-0.12700000
C	2.85500000	-0.78000000	1.28500000
H	2.61200000	-1.83400000	1.18100000
H	2.39800000	-0.36600000	2.18000000
H	3.93100000	-0.63300000	1.30100000

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3 4 1.0 5 1.0 6 1.0
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13 16 2.0
14 16 2.0
15 16 2.0
16 17 1.0
17 18 1.0 19 1.0 20 1.0
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AcNHMe•••$^{-}$$O_2$SMe

optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1

C	2.69500000	-0.39700000	0.01600000
O	3.90600000	-0.16500000	0.06300000
C	2.16400000	-1.80800000	0.00000000
H	1.07900000	-1.83900000	-0.06300000
H	2.59800000	-2.33400000	-0.85000000
H	2.49400000	-2.31400000	0.90600000
N	1.77900000	0.57600000	-0.02300000
C	2.16300000	1.97100000	-0.00500000
H	1.26200000	2.57800000	-0.02500000
H	2.73200000	2.20800000	0.89500000
H	2.78000000	2.21900000	-0.86900000
H	0.79000000	0.33500000	-0.06300000
O	-0.96100000	-0.09300000	-0.13400000
O	-3.15800000	0.44200000	-1.18900000
S	-2.44400000	-0.45500000	-0.19500000
C	-3.02300000	0.21400000	1.38700000
H	-2.76500000	1.27300000	1.38800000
H	-2.52000000	-0.30800000	2.19800000
H	-4.10000000	0.07800000	1.45400000

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3 4 1.0 5 1.0 6 1.0
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7 8 1.0 12 1.0
8 9 1.0 10 1.0 11 1.0
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13 15 1.5
14 15 1.5
15 16 1.0
16 17 1.0 18 1.0 19 1.0
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HOH•••$^{-}$O$_3$SMe
optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1
H -2.10600000 -0.29600000 -0.28200000
O -0.46000000 -0.63200000 -0.88400000
O 0.45900000 -0.59900000 1.38900000
O 1.95600000 -0.40400000 -0.55000000
S 0.62100000 -0.13700000 0.00200000
C 0.43100000 1.63300000 0.04100000
H -0.56200000 1.85600000 0.42200000
H 0.54900000 2.01100000 -0.97100000
H 1.19400000 2.04200000 0.69700000
O -2.99500000 -0.10400000 0.07400000
H -3.28300000 0.69200000 -0.38000000

1 10 1.0
2 5 2.0
3 5 2.0
4 5 2.0
5 6 1.0
6 7 1.0 8 1.0 9 1.0
7
8
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10 11 1.0
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HOH•••$^{-}$O$_2$SMe
optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1
H -1.80400000 -0.24700000 -0.10800000
O -0.38700000 -0.61100000 -0.95400000
O 1.06500000 -0.83000000 1.06700000
S 0.94400000 -0.20700000 -0.31100000
C 0.61700000 1.53000000 0.09300000
H -0.26400000 1.54200000 0.73500000
H 0.43300000 2.07800000 -0.82800000
H 1.48000000 1.93700000 0.61500000
O -2.64500000 -0.05800000 0.37700000
H -2.90900000 0.82000000 0.09100000

1 9 1.0
2 4 1.5
3 4 1.5
4 5 1.0
5 6 1.0 7 1.0 8 1.0
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7
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9 10 1.0
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Mg^{2+}•••$^{-}O_3SMe$
optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1
O -0.44400000 -0.05000000 -1.17600000
O 1.18000000 1.41100000 0.00000000
O -0.44400000 -0.05100000 1.17600000
S 0.47000000 0.15000000 0.00000000
C 1.65500000 -1.15600000 0.00000000
H 2.26100000 -1.03500000 -0.89400000
H 1.12800000 -2.10400000 -0.00100000
H 2.26000000 -1.03600000 0.89400000
Mg -2.12000000 -0.14700000 0.00000000

1 4 2.0 9 1.0
2 4 2.0
3 4 2.0 9 1.0
4 5 1.0 9 1.0
5 6 1.0 7 1.0 8 1.0
6
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Mg^{2+}…$^{-}O_2SMe$
optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1
O 0.30600000 -1.19400000 -0.19900000
O 0.30600000 1.19400000 -0.19900000
S -0.60900000 0.00000000 -0.57600000
C -1.80800000 0.00000000 0.75400000
H -1.25600000 0.00000000 1.69200000
H -2.42000000 -0.89400000 0.65400000
H -2.42000000 0.89400000 0.65300000
Mg 1.81600000 0.00000000 0.40600000

1 3 1.5 8 1.0
2 3 1.5 8 1.0
3 4 1.0 8 1.0
4 5 1.0 6 1.0 7 1.0
5
6
7
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$MeSO_3^-$
optimized M06-2X/aug-cc-pVTZ/H_2O

-1 1
O 0.55595200 -1.15567000 0.81986500
O 0.55320500 1.28816100 0.59193000
O 0.55729600 -0.13115600 -1.41024200
S 0.14942900 0.00020100 0.00000900
C -1.63339000 -0.00148400 -0.00135300
H -1.97464300 0.11783100 1.02321600
H -1.97318100 -0.94894500 -0.41048000
H -1.97432500 0.82611400 -0.61718100

1 4 2.0
2 4 2.0
3 4 2.0
4 5 1.0
5 6 1.0 7 1.0 8 1.0
6
7
8

$MeSO_2^-$
optimized M06-2X/aug-ccp-VTZ/H_2O

-1 1
O -0.72602700 1.24877500 0.29582300
O -0.72599900 -1.24878800 0.29582300
S -0.19866500 -0.00000100 -0.39467400
C 1.53631000 0.00001400 0.13944600
H 1.52716300 0.00002300 1.22952800
H 2.02491200 0.89420100 -0.24230600
H 2.02490500 -0.89418300 -0.24229200

1 3 1.5
2 3 1.5
3 4 1.0
4 5 1.0 6 1.0 7 1.0
5
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AcNHMe
optimized M06-2X/aug-cc-pVTZ/H_2O

0 1
C 0.47676400 0.15178500 0.00015300
O 0.37627300 1.37620500 0.00007300
C 1.81973900 -0.53176500 0.00033900
H 1.74455200 -1.61597400 0.00607200
H 2.37084800 -0.21330600 -0.88282400
H 2.37543200 -0.20395700 0.87711100
N -0.60413600 -0.64592600 -0.00186000
C -1.94830900 -0.10448300 0.00050900
H -2.65502200 -0.92652100 -0.05422800
H -2.13399400 0.46754700 0.90919600
H -2.09570200 0.55310400 -0.85498600
H -0.47650200 -1.64227900 0.00608700

1 2 2.0 3 1.0 7 1.5
2
3 4 1.0 5 1.0 6 1.0
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7 8 1.0 12 1.0
8 9 1.0 10 1.0 11 1.0
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Mg^{2+}
optimized MP2/aug-cc-pVQZ/H_2O
2 1
Mg 0.68149211 -0.15064562 0.00000000

1

H_2O
optimized M062X/aug-cc-pVTZ/H_2O

0 1
O 0.00000000 0.00000000 0.11734800
H 0.00000000 0.76118600 -0.46939100
H 0.00000000 -0.76118600 -0.46939100

1 2 1.0 3 1.0
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Computational analysis of PPII helix model peptides (structures in Figure 20)

A computational study was performed using DFT methods to investigate the impact of cysteine sulfonic acid on the PPII helix structure of a peptide. The study aimed to gain a deeper understanding of the conformational preferences of Cys-SO_3^- within the context of a proline-rich peptide. The peptide Ac-Pro-Pro-Cys(SO_3^-)-Pro-Pro-NMe_2 was chosen as the model for the study. In these models, all proline residues have an *exo* ring pucker and *trans* amide bonds. The geometry optimization calculations were performed using the M06-2X functional and the 6-31+G(d,p) basis set in the implicit H_2O (IEFPCM model). Energies were determined directly from the results of the geometry optimization calculations. The results of the study revealed that the g^- or g^+ rotamers were preferred for PPII, with the PPII conformation in each stabilized by a sulfonate-amide side chain-main chain hydrogen bond. These findings complement the existing experimental data on the relationship between cysteine sulfonic acid and PPII helicity in peptides, allowing for a more thorough understanding of this complex relationship. Additionally, the study showed that the g^- rotamer promotes a more compact conformation at Cys-SO_3^- and a more canonical PPII conformation at Pro_4. In contrast, in the *t* rotamer, a steric clash between the sulfonate and proline caused more distorted PPII conformations at both residues, as well as a non-ideal χ_1 torsion angle. These observations are consistent with the modest PPII propensity of Cys-SO_3^-, with the generally unfavorable nature of the *t* χ_1 rotamer for PPII. The coordinates of the optimized structures are given below.

***g*⁻ Cys(SO_3^-)**

Ac-ProPro-Cys(SO_3^-)-ProPro-NMe_2

optimized M06-2X/6-31+G(d,p)/H_2O

-1 1

C	8.62300000	1.19600000	0.11300000
C	7.48200000	0.26900000	-0.23100000
O	7.09600000	0.09500000	-1.39500000
H	9.49400000	0.61800000	0.43700000
N	6.89100000	-0.38200000	0.79100000
C	5.77800000	-1.28800000	0.52700000
C	4.63600000	-0.55600000	-0.17500000
O	4.23200000	0.52900000	0.25200000
C	5.34800000	-1.74400000	1.93400000
C	6.63400000	-1.61400000	2.75700000
C	7.25800000	-0.32900000	2.21100000
H	6.82200000	0.55900000	2.68500000
H	6.13100000	-2.13300000	-0.06900000
H	4.93500000	-2.75400000	1.92400000
H	7.29900000	-2.46000000	2.55900000
H	8.34300000	-0.29700000	2.33100000
H	4.58900000	-1.05500000	2.31700000
H	6.44800000	-1.56100000	3.83100000
N	4.03100000	-1.17600000	-1.20500000
C	2.83700000	-0.58000000	-1.79300000
C	1.75900000	-0.35900000	-0.73400000
O	1.53200000	-1.18300000	0.15000000
C	2.39800000	-1.62200000	-2.83500000
C	3.72200000	-2.26400000	-3.25700000
C	4.50100000	-2.35900000	-1.94400000
H	4.25400000	-3.27600000	-1.39700000
H	3.08900000	0.37700000	-2.26700000
H	1.84900000	-1.16500000	-3.65900000
H	4.25300000	-1.60600000	-3.95300000
H	5.58000000	-2.30700000	-2.09700000
H	1.75500000	-2.36600000	-2.35200000
H	3.59200000	-3.23800000	-3.73100000
N	1.02300000	0.75700000	-0.89000000
C	-0.01700000	1.06400000	0.06700000
C	-1.07900000	-0.04300000	0.07200000
O	-1.45900000	-0.55600000	-0.98300000
C	-0.74300000	2.35700000	-0.30500000
H	0.42700000	1.18000000	1.06000000
H	-1.50100000	2.58700000	0.44800000
H	-1.22300000	2.27000000	-1.28400000
N	-1.64500000	-0.34700000	1.25300000
C	-2.81600000	-1.21800000	1.26600000
C	-3.93800000	-0.62300000	0.41700000
O	-4.10300000	0.59900000	0.36000000
C	-3.23500000	-1.24400000	2.74900000
C	-1.93000000	-0.94700000	3.49300000
C	-1.24800000	0.08900000	2.59900000
H	-1.62100000	1.10100000	2.80300000
H	-2.53400000	-2.21300000	0.91200000
H	-3.68800000	-2.19800000	3.02600000
H	-1.31100000	-1.84800000	3.54700000
H	-0.16300000	0.07800000	2.70800000
H	-3.96300000	-0.44700000	2.93200000
H	-2.09300000	-0.57500000	4.50600000
N	-4.79000000	-1.47900000	-0.17200000
C	-6.00400000	-0.95300000	-0.79100000
C	-6.83300000	-0.18500000	0.24700000
O	-6.82000000	-0.54600000	1.42600000
C	-6.75100000	-2.21700000	-1.26000000
C	-5.63800000	-3.25400000	-1.43000000
C	-4.69600000	-2.94200000	-0.26700000
H	-5.03900000	-3.41200000	0.66300000
H	-5.72200000	-0.30900000	-1.62800000
H	-7.32200000	-2.04000000	-2.17400000

H	-5.11500000	-3.09800000	-2.37800000
H	-3.67000000	-3.25400000	-0.47100000
H	-7.44400000	-2.54000000	-0.47600000
H	-6.00600000	-4.28100000	-1.40000000
N	-7.60600000	0.82400000	-0.20900000
C	-8.39300000	1.61500000	0.72800000
C	-7.60900000	1.28200000	-1.59600000
H	-8.50900000	1.87900000	-1.75000000
H	-8.04400000	2.65200000	0.72500000
H	-7.64700000	0.44500000	-2.29500000
H	-8.28200000	1.19700000	1.72600000
H	-9.44800000	1.59700000	0.43800000
H	-6.73600000	1.90500000	-1.81700000
H	8.88600000	1.77000000	-0.77400000
H	8.35000000	1.87400000	0.92600000
H	1.33400000	1.50300000	-1.50800000
S	0.35900000	3.78400000	-0.38100000
O	-0.52900000	4.95500000	-0.56100000
O	1.23700000	3.53600000	-1.55900000
O	1.10000000	3.78700000	0.90200000

1 2 1.0 4 1.0 78 1.0 79 1.0
2 3 2.0 5 1.5
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5 6 1.0 11 1.0
6 7 1.0 9 1.0 13 1.0
7 8 2.0 19 1.5
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9 10 1.0 14 1.0 17 1.0
10 11 1.0 15 1.0 18 1.0
11 12 1.0 16 1.0
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19 20 1.0 25 1.0
20 21 1.0 23 1.0 27 1.0
21 22 2.0 33 1.5
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23 24 1.0 28 1.0 31 1.0
24 25 1.0 29 1.0 32 1.0
25 26 1.0 30 1.0
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33 34 1.0 80 1.0
34 35 1.0 37 1.0 38 1.0
35 36 2.0 41 1.5
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37 39 1.0 40 1.0 81 1.0
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41 42 1.0 47 1.0
42 43 1.0 45 1.0 49 1.0
43 44 2.0 55 1.5
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45 46 1.0 50 1.0 53 1.0
46 47 1.0 51 1.0 54 1.0
47 48 1.0 52 1.0
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55 56 1.0 61 1.0
56 57 1.0 59 1.0 63 1.0
57 58 2.0 69 1.5
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81 82 2.0 83 2.0 84 2.0
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***g*⁺ Cys(SO_3^-)**

Ac-ProPro-Cys(SO_3^-)-ProPro-NMe_2

optimized M06-2X/6-31+G(d,p)/H_2O

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C	8.90400000	-0.72500000	1.17300000
C	7.65200000	0.08900000	0.95400000
O	6.99000000	0.55200000	1.89300000
H	9.78500000	-0.15300000	0.86500000
N	7.27700000	0.30600000	-0.32300000
C	6.07200000	1.08300000	-0.60200000
C	4.84700000	0.43800000	0.04400000
O	4.64000000	-0.77200000	-0.08200000
C	5.96200000	1.03300000	-2.13700000
C	7.41100000	0.83000000	-2.59300000
C	7.96700000	-0.13000000	-1.54100000
H	7.71000000	-1.17100000	-1.77500000
H	6.21300000	2.10800000	-0.24800000
H	5.49900000	1.93600000	-2.53900000
H	7.95900000	1.77700000	-2.55300000
H	9.05000000	-0.05300000	-1.42400000
H	5.35600000	0.16800000	-2.42400000
H	7.48600000	0.42700000	-3.60400000
N	3.96600000	1.24400000	0.66300000
C	2.70300000	0.69000000	1.13600000
C	1.91600000	0.04500000	-0.00100000
O	1.90700000	0.51600000	-1.13700000
C	1.95900000	1.92000000	1.68500000
C	3.09700000	2.83000000	2.15400000
C	4.15800000	2.64600000	1.06700000
H	3.98200000	3.31900000	0.21900000
H	2.88800000	-0.05100000	1.92400000
H	1.25500000	1.65000000	2.47300000
H	3.48900000	2.47900000	3.11400000
H	5.17100000	2.79700000	1.44500000
H	1.40700000	2.39900000	0.86900000
H	2.79300000	3.87200000	2.26200000
N	1.19000000	-1.03500000	0.35600000
C	0.20200000	-1.57000000	-0.54900000
C	-1.00400000	-0.60900000	-0.65100000
O	-1.14800000	0.32000000	0.14400000
C	-0.15500000	-3.01300000	-0.18200000
H	0.66700000	-1.60100000	-1.54100000
H	0.74900000	-3.62500000	-0.21200000
H	-0.88200000	-3.42800000	-0.88400000
N	-1.85500000	-0.78900000	-1.68300000
C	-2.88100000	0.23200000	-1.93700000
C	-3.96500000	0.22300000	-0.86000000
O	-4.62000000	-0.80400000	-0.64900000
C	-3.47000000	-0.17100000	-3.30100000
C	-2.34600000	-0.97500000	-3.96100000
C	-1.76400000	-1.75600000	-2.78500000
H	-2.37500000	-2.64000000	-2.56200000
H	-2.39000000	1.20800000	-1.99200000
H	-3.77800000	0.70200000	-3.87800000
H	-1.58300000	-0.30600000	-4.37200000
H	-0.73400000	-2.07300000	-2.95600000
H	-4.34100000	-0.81300000	-3.13700000
H	-2.70400000	-1.63000000	-4.75800000
N	-4.22900000	1.37000000	-0.21000000
C	-5.34300000	1.39800000	0.73200000
C	-6.66100000	1.08700000	0.01100000
O	-6.80800000	1.41800000	-1.16800000
C	-5.32500000	2.83900000	1.27100000
C	-3.85600000	3.24600000	1.13200000
C	-3.44600000	2.61500000	-0.19900000
H	-3.72900000	3.25100000	-1.04600000
H	-5.15000000	0.66600000	1.52200000
H	-5.70100000	2.90200000	2.29400000
H	-3.26500000	2.80700000	1.94200000

H	-2.38100000	2.38700000	-0.24300000
H	-5.95000000	3.47200000	0.63100000
H	-3.71000000	4.32800000	1.14100000
N	-7.63700000	0.51000000	0.74400000
C	-8.89600000	0.13800000	0.11400000
C	-7.47800000	0.10100000	2.13700000
H	-8.47200000	0.00300000	2.57400000
H	-9.04400000	-0.94400000	0.19400000
H	-6.93700000	0.85100000	2.71500000
H	-8.86900000	0.42400000	-0.93500000
H	-9.72900000	0.64400000	0.61100000
H	-6.96500000	-0.86400000	2.21700000
H	8.98600000	-0.96000000	2.23400000
H	8.88500000	-1.65000000	0.59100000
H	1.12100000	-1.31400000	1.33100000
S	-0.86200000	-3.25500000	1.46200000
O	-0.94400000	-4.72600000	1.61700000
O	-2.18200000	-2.58800000	1.45300000
O	0.10000000	-2.62500000	2.41000000

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***t* Cys(SO_3^-)**

Ac-ProPro-Cys(SO_3^-)-ProPro-NMe_2

optimized M06-2X/6-31+G(d,p)/H_2O

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C	-8.76800000	-0.70700000	-1.19700000
C	-7.59700000	0.18800000	-0.86700000
O	-7.12200000	0.98400000	-1.68700000
H	-9.65200000	-0.40400000	-0.62800000
N	-7.08500000	0.09300000	0.37700000
C	-5.93600000	0.90800000	0.75300000
C	-4.74400000	0.61900000	-0.15700000
O	-4.48100000	-0.53800000	-0.49600000
C	-5.62700000	0.45600000	2.19500000
C	-6.97200000	-0.08000000	2.70000000
C	-7.54600000	-0.77500000	1.46500000
H	-7.13300000	-1.78500000	1.34900000
H	-6.21400000	1.96500000	0.71700000
H	-5.22700000	1.27300000	2.79900000
H	-7.62500000	0.74800000	2.99400000
H	-8.63500000	-0.83800000	1.47900000
H	-4.89000000	-0.35300000	2.16900000
H	-6.86600000	-0.75800000	3.54800000
N	-3.94300000	1.64900000	-0.48900000
C	-2.70400000	1.38300000	-1.21000000
C	-1.83500000	0.37900000	-0.46000000
O	-1.72000000	0.39700000	0.76400000
C	-2.02100000	2.76100000	-1.26800000
C	-3.20200000	3.73400000	-1.25700000
C	-4.17800000	3.08600000	-0.27500000
H	-3.94900000	3.36200000	0.76100000
H	-2.92800000	1.00200000	-2.21500000
H	-1.37700000	2.85900000	-2.14400000
H	-3.65800000	3.78500000	-2.25100000
H	-5.21600000	3.34400000	-0.49400000
H	-1.41300000	2.89900000	-0.36700000
H	-2.91900000	4.74300000	-0.95300000
N	-1.14400000	-0.48400000	-1.23500000
C	-0.13200000	-1.34400000	-0.64300000
C	1.05000000	-0.45700000	-0.20900000
O	1.57200000	0.29600000	-1.04200000
C	0.30100000	-2.39400000	-1.66600000
H	-0.59100000	-1.84300000	0.21300000
H	1.12200000	-2.03500000	-2.29300000
H	-0.54300000	-2.67600000	-2.29900000
N	1.46100000	-0.49300000	1.06400000
C	2.51200000	0.43200000	1.50600000
C	3.77700000	0.33200000	0.65300000
O	4.37400000	-0.74200000	0.53600000
C	2.77900000	-0.01200000	2.94900000
C	1.41400000	-0.52600000	3.41100000
C	0.87900000	-1.26000000	2.17900000
H	1.22800000	-2.29600000	2.12700000
H	2.11300000	1.45200000	1.48600000
H	3.17000000	0.80500000	3.55900000
H	0.75800000	0.31500000	3.65600000
H	-0.21000000	-1.23100000	2.12600000
H	3.50900000	-0.82800000	2.93700000
H	1.47700000	-1.18000000	4.28200000
N	4.26900000	1.46600000	0.12300000
C	5.53600000	1.40400000	-0.59800000
C	6.66300000	0.94100000	0.33200000
O	6.64000000	1.24700000	1.52600000
C	5.75000000	2.85300000	-1.06600000
C	4.32200000	3.37900000	-1.22800000
C	3.58400000	2.75700000	-0.04100000
H	3.69400000	3.36800000	0.86300000
H	5.42400000	0.71900000	-1.44400000
H	6.34200000	2.90800000	-1.98200000
H	3.89100000	3.00900000	-2.16400000

H	2.52500000	2.59600000	-0.25000000
H	6.27000000	3.41300000	-0.28000000
H	4.26400000	4.46900000	-1.22600000
N	7.68100000	0.25900000	-0.23700000
C	8.76600000	-0.25100000	0.59100000
C	7.72000000	-0.12400000	-1.64600000
H	8.75200000	-0.37200000	-1.89700000
H	8.81300000	-1.34200000	0.50800000
H	7.41300000	0.69900000	-2.29300000
H	8.58400000	0.02500000	1.62700000
H	9.72000000	0.16900000	0.26100000
H	7.09300000	-1.00000000	-1.84400000
H	-8.98300000	-0.62200000	-2.26100000
H	-8.55000000	-1.74900000	-0.94700000
H	-1.17700000	-0.38600000	-2.24200000
S	0.83500000	-3.92200000	-0.87100000
O	1.26200000	-4.80100000	-1.98600000
O	-0.36000000	-4.42700000	-0.15000000
O	1.93800000	-3.54200000	0.04300000

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Computational analysis of α-helix model peptides (structures from Figure 21)

To further understand the experimental data about the effect of cysteine sulfonate and other cysteine oxoforms and ionization states on α-helicity, an examination of the geometry of minimal α-helical model (Ac-Ala-X-Ala_9-NHMe, X= Cys-SH, Cys-S^-, Cys-SO_2^-, and Cys-SO_3^-) was conducted, taking into account the nuances of the rotameric states (g^-, g^+, and t) of the cysteine side-chain, as well as its ionization and oxidation state. To achieve this, a detailed iterative geometry optimization process was initiated, utilizing an initial geometry-optimized Ac-Ala_{11}-NHMe model in an α-helical conformation as the starting point. The cysteine side chains were incorporated using the Builder function in GaussView 5, and the side chain was rotated into the examined rotamer. The geometry optimization procedure was performed on all structures using the M11-L DFT functional and the Def2SVP basis set. Additionally, implicit water was taken into consideration by utilizing the IEFPCM model. All geometry optimization calculations terminated normally. Energies were determined directly from the geometry optimization calculations. The coordinates of the geometry-optimized structures are given below.

***g*⁻ Cys-SH**

Ac-Ala-Cys-SH-Ala$_9$-NHMe

optimized M11L/Def2SVP/H_2O

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C	-8.86200800	-2.49288500	1.35987000
H	-9.89179000	-2.37522500	0.99154200
C	-7.82123900	-2.04849400	0.39885300
O	-6.63591100	-2.04525600	0.67764600
N	-8.23169500	-1.62338900	-0.80079300
H	-9.20876200	-1.70576700	-1.05808100
C	-7.26924200	-1.31457600	-1.81023700
H	-6.61958900	-2.19879800	-1.99628600
C	-7.94109800	-0.90464700	-3.09367700
C	-6.30424400	-0.23832200	-1.34365600
H	-8.57509000	-0.01016300	-2.95641600
H	-7.18920200	-0.67209800	-3.86417500
H	-8.57469400	-1.71997300	-3.48281600
O	-5.13870100	-0.25247700	-1.66733700
N	-6.81255600	0.74444900	-0.59590300
H	-7.81226200	0.79030500	-0.41841000
C	-5.96435300	1.81788600	-0.19123900
H	-5.44297400	2.24198900	-1.07892200
C	-6.74869900	2.90584700	0.50034800
C	-4.84484800	1.33374500	0.72826600
H	-7.24588300	2.50291000	1.40529700
H	-6.04401100	3.69123100	0.83065300
O	-3.74876500	1.84565600	0.70626000
N	-5.18517600	0.36577000	1.57588100
H	-6.07071600	-0.11883600	1.44968200
C	-4.21482400	-0.20727500	2.45616700
H	-3.64079200	0.61600700	2.92978100
C	-4.87780500	-1.04757300	3.51474100
C	-3.17328700	-1.00567800	1.68008100
H	-5.47153100	-1.86396900	3.06482900
H	-4.12363700	-1.49940000	4.17924300
H	-5.55208100	-0.43391500	4.13627300
O	-1.99549700	-0.96191500	1.96416200
N	-3.63747200	-1.75189500	0.68044200
H	-4.63971000	-1.80892500	0.49588000
C	-2.71824300	-2.47727000	-0.13680500
H	-2.08020100	-3.12682700	0.50107600
C	-3.45304800	-3.31299900	-1.15044400
C	-1.73688800	-1.52060500	-0.81002800
H	-4.07421800	-2.68242300	-1.81361100
H	-2.74509600	-3.87663800	-1.77938300
H	-4.11191600	-4.04394300	-0.64997700
O	-0.55627600	-1.77932300	-0.90609600
N	-2.27223300	-0.40679400	-1.30434500
H	-3.28427900	-0.27428500	-1.28738500
C	-1.45191000	0.55393900	-1.96894800
H	-0.83911100	0.04970100	-2.74828600
C	-2.30235700	1.62494400	-2.60052100
C	-0.42672100	1.15754100	-1.01512200
H	-2.91640800	2.14681800	-1.84237500
H	-1.67307100	2.37458900	-3.10721600
H	-2.98339400	1.19089100	-3.35312000
O	0.71586500	1.36843800	-1.36355000
N	-0.86881100	1.45561200	0.20320800
H	-1.85920300	1.36274800	0.43241100
C	0.02693600	2.00001800	1.17170100
H	0.53732600	2.89654800	0.75556800
C	-0.71744100	2.36878000	2.42785200
C	1.16148800	1.02417600	1.47133600
H	-1.21813100	1.48436300	2.86471900
H	-0.02972200	2.78318500	3.18309400
H	-1.48863000	3.13021500	2.21762900
O	2.30010000	1.40823400	1.63905500
N	0.81090600	-0.25539400	1.56437900
H	-0.17112400	-0.52677700	1.48974800

C	1.79953900	-1.25181500	1.82531300
H	2.41314400	-0.94572500	2.70081800
C	1.15137300	-2.58490000	2.09090900
C	2.80192400	-1.34609400	0.67779900
H	0.54816000	-2.91265900	1.22377300
H	1.91333700	-3.35548000	2.29323600
H	0.48514700	-2.52886400	2.96949500
O	3.98937100	-1.48831600	0.87969600
N	2.28714700	-1.28290100	-0.54672600
H	1.27595700	-1.23939500	-0.68453700
C	3.15416900	-1.32261100	-1.67924500
H	3.80708200	-2.22155800	-1.62318000
C	2.35592300	-1.34393600	-2.95546900
C	4.12810900	-0.14518100	-1.65765300
H	1.70845600	-0.45048300	-3.03171800
H	3.02316500	-1.36319400	-3.83299100
H	1.71122300	-2.23927200	-3.00304300
O	5.29309600	-0.26847600	-1.96513100
N	3.59973700	1.02538900	-1.30141700
H	2.59972800	1.10795800	-1.11135000
C	4.43376500	2.18038200	-1.22958000
H	4.98356100	2.30931500	-2.18750200
C	3.61410600	3.41013900	-0.94011600
C	5.53785700	1.99334200	-0.19069400
H	3.06871500	3.30968200	0.01675400
H	4.25807300	4.30307400	-0.87755700
H	2.87229300	3.58423200	-1.73952000
O	6.68313900	2.32656200	-0.40325900
N	5.15119900	1.45788400	0.96709500
H	4.16710000	1.24189100	1.13626300
C	6.10661200	1.23446500	2.00223600
H	6.65398700	2.17794600	2.22175200
C	5.42304600	0.74304200	3.25159600
C	7.20629700	0.26273300	1.57563000
H	4.89185300	-0.20860600	3.06098400
H	6.15748900	0.57479900	4.05650800
H	4.68520500	1.48032000	3.61472400
O	8.32776200	0.34920600	2.01697800
N	6.82283200	-0.69186100	0.72480100
H	5.83600100	-0.78187900	0.48173700
C	7.74154000	-1.67698500	0.26120400
H	8.37587500	-2.01244300	1.11104900
C	7.00298800	-2.85857000	-0.31314200
C	8.74800600	-1.15137100	-0.76086200
H	6.36455400	-2.54248500	-1.15959400
H	7.71313500	-3.61934700	-0.67647900
H	6.35425600	-3.32758100	0.44715200
O	9.76885900	-1.76745300	-0.97340600
N	8.39702500	-0.03443200	-1.39120000
H	7.50161800	0.39151400	-1.16519300
C	9.19994200	0.57367700	-2.38561000
H	8.77783300	0.45364200	-3.40326800
H	-8.74850600	-1.92982200	2.30036400
H	-8.69180100	-3.55381400	1.60702100
H	10.19906700	0.10939800	-2.37886600
H	9.31409200	1.65720600	-2.20011200
S	-7.97797300	3.58344000	-0.63521500
H	-8.57517300	4.37973400	0.27250800

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***g*$^+$ Cys-SH**

Ac-Ala-Cys-SH-Ala$_9$-NHMe

optimized M11L/Def2SVP/H_2O

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C	-9.00920600	-0.98314600	2.16697500
H	-10.01256500	-1.22759400	1.78825100
C	-7.90821200	-1.33761000	1.23617200
O	-6.73452700	-1.19193200	1.52882800
N	-8.24783900	-1.79118600	0.02499800
H	-9.21990600	-1.98219600	-0.19115500
C	-7.22925500	-2.20901600	-0.88483300
H	-6.59291600	-2.98329500	-0.40109800
C	-7.82180200	-2.76626800	-2.15114400
C	-6.26203600	-1.07963900	-1.19859900
H	-8.45014600	-2.01931100	-2.66873200
H	-7.02287100	-3.07644100	-2.84299000
H	-8.44200300	-3.65387100	-1.93870400
O	-5.10077300	-1.30717900	-1.45701800
N	-6.76644600	0.15306500	-1.21932000
H	-7.74064200	0.31281700	-0.97441600
C	-5.92985700	1.27276800	-1.48624300
H	-5.36355600	1.10508800	-2.42742000
C	-6.75018200	2.53226100	-1.66942900
C	-4.85196500	1.46501500	-0.42229800
H	-6.06376300	3.37958000	-1.85129400
H	-7.38349900	2.43303900	-2.56807300
O	-3.75720400	1.89322200	-0.71371700
N	-5.21614100	1.18198700	0.82631400
H	-6.09876600	0.70326400	0.99455700
C	-4.27075100	1.25737400	1.89527600
H	-3.69250900	2.19813600	1.78580200
C	-4.96322200	1.23050900	3.23143400
C	-3.22790600	0.15152400	1.77610500
H	-5.56625500	0.31251600	3.35227000
H	-4.22688600	1.26973400	4.05035800
H	-5.63468000	2.09956200	3.33761200
O	-2.05943200	0.34819900	2.03237200
N	-3.67802100	-1.03419700	1.37118300
H	-4.67509600	-1.18384900	1.21461000
C	-2.74921600	-2.09651800	1.14860600
H	-2.12540200	-2.24277400	2.05696800
C	-3.46638500	-3.37496900	0.80752200
C	-1.74855100	-1.70787900	0.06012900
H	-4.07090200	-3.26290200	-0.11139900
H	-2.74682500	-4.19388900	0.64521900
H	-4.13745900	-3.67860800	1.63011300
O	-0.56875100	-1.96972300	0.15786100
N	-2.26266800	-1.08270900	-0.99657200
H	-3.27513400	-0.98723200	-1.09074600
C	-1.41718200	-0.67948100	-2.07388600
H	-0.79973100	-1.54115300	-2.41126200
C	-2.23665200	-0.15751100	-3.22465000
C	-0.39861600	0.35604400	-1.60852100
H	-2.85099300	0.70943800	-2.91658400
H	-1.58409300	0.16265500	-4.05330200
H	-2.91325600	-0.93995000	-3.61036400
O	0.75290700	0.32999300	-1.98918800
N	-0.85644800	1.29000800	-0.77927500
H	-1.85251100	1.34593800	-0.56283900
C	0.03490000	2.27781500	-0.26425400
H	0.57262700	2.77406500	-1.10197300
C	-0.71782200	3.30484200	0.53967900
C	1.14200800	1.63299400	0.56402500
H	-1.24085100	2.83699500	1.39472000
H	-0.03092100	4.07117400	0.93472800
H	-1.47019500	3.81634300	-0.08567300
O	2.28600500	2.03367600	0.50994600
N	0.76619100	0.63877100	1.36286200
H	-0.21768100	0.37249500	1.43132600

C	1.73443600	-0.03252000	2.16966400
H	2.33142200	0.71670700	2.73501300
C	1.06146500	-0.98062100	3.12657300
C	2.76264700	-0.75936800	1.30547600
H	0.46612100	-1.73679600	2.58178100
H	1.80824000	-1.50691100	3.74325100
H	0.38388000	-0.43584700	3.80699100
O	3.93925200	-0.78271000	1.59778800
N	2.27646500	-1.37552800	0.23147400
H	1.27022200	-1.39225800	0.05677500
C	3.16223700	-2.05250900	-0.65987200
H	3.79577400	-2.76790900	-0.09058600
C	2.38273400	-2.78522500	-1.71990900
C	4.15730900	-1.07530900	-1.28223200
H	1.75975600	-2.08405400	-2.30575800
H	3.06110000	-3.30830400	-2.41381200
H	1.71610200	-3.53966300	-1.26633700
O	5.33041400	-1.34708400	-1.41285900
N	3.64003100	0.08307600	-1.69113400
H	2.63759000	0.26305900	-1.61491300
C	4.49586000	1.07237600	-2.26016600
H	5.07157200	0.63657400	-3.10565600
C	3.69083900	2.25160200	-2.73901100
C	5.56660200	1.50679000	-1.26174100
H	3.12184900	2.70589100	-1.90641700
H	4.34604400	3.02554100	-3.17197700
H	2.97055500	1.94572500	-3.51819200
O	6.72349700	1.66394100	-1.58534900
N	5.13236700	1.72631000	-0.02099300
H	4.13855800	1.64640100	0.20135900
C	6.04352800	2.16389200	0.98492300
H	6.58412500	3.07193100	0.63692400
C	5.30719000	2.46802200	2.26332600
C	7.15429700	1.14672400	1.23654000
H	4.77788400	1.57002200	2.63415200
H	6.00775100	2.80495100	3.04508500
H	4.56005300	3.26666200	2.10956800
O	8.26412900	1.49188300	1.56697600
N	6.79272600	-0.13171600	1.10513600
H	5.81565200	-0.36382000	0.92595900
C	7.72462200	-1.18280500	1.33825600
H	8.30981500	-0.95703100	2.25685300
C	7.00695300	-2.49685700	1.50846100
C	8.78838000	-1.31456200	0.25079300
H	6.42339200	-2.74144400	0.60082900
H	7.72864500	-3.31038100	1.68774100
H	6.30870000	-2.45915100	2.36284300
O	9.82495500	-1.89362800	0.48885400
N	8.46451900	-0.80483000	-0.93450500
H	7.56000600	-0.35110100	-1.04027200
C	9.32818600	-0.85363700	-2.05506900
H	8.92196700	-1.48331200	-2.87026400
H	-8.96338400	0.09965400	2.37418200
H	-8.84951500	-1.49580400	3.12904100
H	10.29470000	-1.28137700	-1.74452100
H	9.51018800	0.15416800	-2.47273700
S	-7.81354300	2.88960800	-0.24222100
H	-8.95187100	3.03316000	-0.94549100

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***t* Cys-SH**

Ac-Ala-Cys-SH-Ala_9-NHMe

optimized M11L/Def2SVP/H_2O

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C	-8.96001100	-2.07002100	1.85077100
H	-9.97720200	-2.09611000	1.43306100
C	-7.89156600	-1.91977800	0.83037100
O	-6.71597700	-1.81613700	1.12961400
N	-8.26761900	-1.87853200	-0.45249100
H	-9.23612400	-2.04734300	-0.69989300
C	-7.27716000	-1.87200900	-1.48174200
H	-6.60234900	-2.74842900	-1.35813800
C	-7.91279900	-1.91937100	-2.84561200
C	-6.34930000	-0.67627500	-1.35818000
H	-8.57858300	-1.05446000	-3.01699900
H	-7.14043100	-1.91617000	-3.63058200
H	-8.50758800	-2.84069500	-2.96678200
O	-5.18359100	-0.75353700	-1.67336600
N	-6.88560300	0.46696800	-0.92580600
H	-7.87880600	0.51493600	-0.72108000
C	-6.06211200	1.62739400	-0.82946600
H	-5.53083600	1.79240700	-1.79288600
C	-6.91594400	2.83551500	-0.51847700
C	-4.94756300	1.43299600	0.19771900
H	-7.69388900	2.92400700	-1.30119500
H	-7.43322200	2.69536200	0.45258600
O	-3.84072000	1.88740700	0.01318900
N	-5.29231800	0.77898300	1.30511800
H	-6.17928000	0.28205700	1.33545900
C	-4.31336900	0.48862800	2.30495500
H	-3.73960900	1.41595500	2.51194900
C	-4.96296200	-0.00592200	3.56958500
C	-3.27086600	-0.49742600	1.79033700
H	-5.56365000	-0.91491800	3.38320700
H	-4.19981100	-0.24897800	4.32630500
H	-5.62697500	0.76579400	3.99494500
O	-2.09888300	-0.38952100	2.08239600
N	-3.72305500	-1.47792800	1.01248200
H	-4.72294600	-1.58492600	0.83819000
C	-2.79426200	-2.40334700	0.44662600
H	-2.16292400	-2.83731300	1.25234600
C	-3.51407700	-3.50025000	-0.29072700
C	-1.80178900	-1.67705600	-0.45966500
H	-4.11389200	-3.09442400	-1.12618900
H	-2.79770700	-4.22749100	-0.70627000
H	-4.19117300	-4.04745500	0.38847800
O	-0.62392000	-1.96486500	-0.46926600
N	-2.31954300	-0.73420900	-1.24337700
H	-3.32909900	-0.58371000	-1.26478500
C	-1.48035200	0.00811400	-2.12886800
H	-0.85426400	-0.69285900	-2.72326300
C	-2.31108700	0.86224000	-3.04976900
C	-0.47218700	0.85137900	-1.35505500
H	-2.93509600	1.57532800	-2.47863200
H	-1.66763800	1.44015000	-3.73313000
H	-2.98078000	0.23686700	-3.66562300
O	0.67550600	0.97186400	-1.72904000
N	-0.93433700	1.45564400	-0.26421700
H	-1.92737200	1.41345200	-0.03004900
C	-0.05202100	2.24392600	0.53455600
H	0.46778100	2.99231000	-0.10344500
C	-0.81218800	2.94102900	1.63139800
C	1.07389500	1.38408800	1.10481700
H	-1.32118000	2.20964500	2.28688600
H	-0.13234300	3.54564800	2.25364100
H	-1.57784100	3.61606400	1.21075600
O	2.21339800	1.79398000	1.17865900
N	0.70928500	0.17999800	1.53566900
H	-0.27497400	-0.09292600	1.51815800

C	1.67966500	-0.71171500	2.08374100
H	2.28369400	-0.17683400	2.84912900
C	1.01071900	-1.91126800	2.70058100
C	2.69941500	-1.13065100	1.02681600
H	0.41902900	-2.46701400	1.94915700
H	1.76046300	-2.59801100	3.12673900
H	0.33004400	-1.60512200	3.51396900
O	3.88173400	-1.22000600	1.28155000
N	2.20243900	-1.40432000	-0.17634100
H	1.19406500	-1.38601000	-0.33870500
C	3.08357300	-1.76335100	-1.23995700
H	3.72389600	-2.61806300	-0.92825100
C	2.30116300	-2.12745000	-2.47354500
C	4.07221800	-0.63526700	-1.52557800
H	1.67301200	-1.28043500	-2.80779300
H	2.97921800	-2.40102600	-3.29866900
H	1.63886700	-2.98951500	-2.28052200
O	5.24361400	-0.84588800	-1.74842100
N	3.55226700	0.59286200	-1.53267800
H	2.55018000	0.73726500	-1.39900100
C	4.40767100	1.71107100	-1.76517100
H	4.97138600	1.56710300	-2.71268900
C	3.60977000	2.98617700	-1.83213700
C	5.49381500	1.79404200	-0.69606200
H	3.05828500	3.16159900	-0.88964100
H	4.26963300	3.85104100	-2.01173200
H	2.87513800	2.94559800	-2.65553700
O	6.65041600	2.03209900	-0.97039200
N	5.08036200	1.61272000	0.55731800
H	4.09024200	1.46241600	0.75982400
C	6.01533000	1.69122900	1.63166700
H	6.55966600	2.66085600	1.58815000
C	5.30830400	1.56773200	2.95608000
C	7.12207500	0.64433700	1.51598300
H	4.77481200	0.60142400	3.02808300
H	6.02964000	1.62914500	3.78746200
H	4.56928400	2.37799700	3.08721600
O	8.23256000	0.85590900	1.94203500
N	6.75245800	-0.50901300	0.95483000
H	5.77300300	-0.65471900	0.71030500
C	7.66491900	-1.59078200	0.79876800
H	8.32139100	-1.63431400	1.69571500
C	6.92225000	-2.89405500	0.65573700
C	8.64317100	-1.42656300	-0.36273700
H	6.25837100	-2.86568100	-0.22916300
H	7.63068700	-3.72889100	0.53146000
H	6.29891700	-3.09541700	1.54409600
O	9.59654500	-2.16931800	-0.44951400
N	8.35780400	-0.46413100	-1.23418500
H	7.50959800	0.08242600	-1.10519900
C	9.15827700	-0.19771700	-2.37102200
H	8.67154900	-0.51493700	-3.31452800
H	-8.88754700	-1.24092800	2.57326200
H	-8.78329500	-2.99764900	2.41964100
H	10.10939500	-0.74593100	-2.28046100
H	9.38197300	0.88097800	-2.45932000
S	-5.90796700	4.32914000	-0.48374100
H	-6.95546100	5.15772000	-0.31443600

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***g*⁻ Cys-S⁻**
Ac-Ala-Cys-S⁻-Ala$_9$-NHMe
optimized M11L/Def2SVP/H_2O

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C	-8.80668700	-2.43639300	1.41045400
H	-9.84879700	-2.31328200	1.07956200
C	-7.79423100	-2.02932000	0.40043100
O	-6.59926200	-2.07165700	0.63071600
N	-8.24811600	-1.59480500	-0.77691400
H	-9.24268000	-1.61191700	-0.97039300
C	-7.33816000	-1.25764100	-1.82591100
H	-6.75417300	-2.15554200	-2.12749100
C	-8.07778300	-0.70648000	-3.01691100
C	-6.29863800	-0.25366100	-1.34708600
H	-8.60806800	0.23234400	-2.76676900
H	-7.37532900	-0.48619300	-3.83678900
H	-8.81756900	-1.43149600	-3.39904200
O	-5.13199400	-0.35605400	-1.66435200
N	-6.76875900	0.74148200	-0.60329100
H	-7.76807900	0.98322800	-0.61785300
C	-5.93575500	1.83375100	-0.23265200
H	-5.43765600	2.27391500	-1.12625100
C	-6.80669500	2.90991000	0.42221800
C	-4.82967600	1.37370900	0.69281400
H	-7.09129400	2.53115600	1.43476600
H	-6.13756800	3.77606500	0.62102800
O	-3.72431500	1.87624500	0.68279700
N	-5.17710100	0.42603500	1.56771100
H	-6.06934000	-0.04492000	1.44155500
C	-4.21791300	-0.14039500	2.45928200
H	-3.64434900	0.68199300	2.93589700
C	-4.89303100	-0.97571900	3.51482200
C	-3.17038400	-0.94875300	1.70169700
H	-5.48506500	-1.79086300	3.05918400
H	-4.14854900	-1.43017300	4.18882300
H	-5.57268900	-0.35903100	4.12772600
O	-1.99607800	-0.91523800	2.00523100
N	-3.62860100	-1.69885200	0.70274900
H	-4.62708600	-1.72668300	0.49046200
C	-2.70884000	-2.43194300	-0.10525900
H	-2.05500800	-3.05135200	0.54640600
C	-3.43900700	-3.31281300	-1.08343200
C	-1.74349000	-1.48426300	-0.81344500
H	-4.08872800	-2.71677200	-1.75075900
H	-2.72661600	-3.87626000	-1.70781100
H	-4.07052500	-4.04515100	-0.55086300
O	-0.56287600	-1.74352400	-0.92030300
N	-2.28545500	-0.37826700	-1.31550400
H	-3.29930900	-0.24725400	-1.29069400
C	-1.46888000	0.58136300	-1.98651500
H	-0.85757100	0.07597900	-2.76642300
C	-2.32353200	1.64956300	-2.61741500
C	-0.44061900	1.18856300	-1.03661300
H	-2.93320100	2.17340100	-1.85714400
H	-1.69790300	2.39706400	-3.13198800
H	-3.00938300	1.21155200	-3.36350300
O	0.70530700	1.38714600	-1.38302200
N	-0.88402600	1.49960900	0.17795500
H	-1.87893500	1.42864100	0.40269800
C	0.01615500	2.04401600	1.14200700
H	0.52911200	2.93822500	0.72341600
C	-0.72186500	2.41778200	2.40060700
C	1.14824400	1.06491700	1.43973800
H	-1.22254800	1.53565000	2.84190300
H	-0.02960800	2.83346200	3.15113200
H	-1.49299200	3.17954600	2.19156400
O	2.29048700	1.44482100	1.59507700
N	0.79310500	-0.21211300	1.54573400
H	-0.19167000	-0.47990200	1.48761100

C	1.78065200	-1.20963900	1.80613900
H	2.39824800	-0.90258900	2.67881500
C	1.13116200	-2.54090200	2.07768600
C	2.77883800	-1.31039500	0.65558800
H	0.52572600	-2.86949000	1.21250300
H	1.89271300	-3.31180300	2.28050500
H	0.46644400	-2.48144900	2.95717500
O	3.96541800	-1.46537800	0.85400600
N	2.26210000	-1.23867100	-0.56727600
H	1.25087300	-1.18602400	-0.70313700
C	3.12755700	-1.28473800	-1.70045300
H	3.76810000	-2.19298500	-1.64925100
C	2.33066400	-1.28838900	-2.97762500
C	4.11942000	-0.12254700	-1.67126000
H	1.69715200	-0.38501300	-3.05080300
H	2.99929300	-1.31497200	-3.85396900
H	1.67226100	-2.17343600	-3.02987300
O	5.28303000	-0.26089400	-1.97533700
N	3.60924600	1.05547400	-1.30936000
H	2.61175300	1.15215200	-1.11259200
C	4.46810500	2.19114300	-1.21760600
H	5.03305600	2.31337700	-2.16736800
C	3.67272600	3.43707900	-0.92936200
C	5.55547500	1.97183300	-0.16744300
H	3.11044800	3.34083600	0.01807000
H	4.33519000	4.31493000	-0.84925000
H	2.94798100	3.63488200	-1.73880800
O	6.71255200	2.27766100	-0.36578500
N	5.14579800	1.44204200	0.98357000
H	4.15566600	1.24265400	1.13969900
C	6.08317400	1.19771500	2.03116000
H	6.63844800	2.13305200	2.26542700
C	5.37521200	0.70672700	3.26682700
C	7.17867800	0.21519600	1.61807600
H	4.83663800	-0.23748800	3.06110500
H	6.09654400	0.52497100	4.08051300
H	4.64091000	1.45012700	3.62449600
O	8.28120700	0.26599400	2.10964400
N	6.80800300	-0.70090700	0.72139200
H	5.82923800	-0.75299700	0.43834000
C	7.70438200	-1.70101200	0.24858300
H	8.36850700	-2.00562400	1.08781700
C	6.94263000	-2.90288700	-0.24690500
C	8.67595600	-1.22048900	-0.82703000
H	6.25751800	-2.61678400	-1.06733400
H	7.63770300	-3.66983100	-0.62439300
H	6.33651800	-3.34802300	0.56072900
O	9.57383000	-1.94961400	-1.18818500
N	8.45912100	-0.00134100	-1.30999700
H	7.64967700	0.52232600	-0.98406400
C	9.26925700	0.57677500	-2.31694600
H	8.76584800	0.60126500	-3.30387100
H	-8.65202400	-1.84931600	2.33069500
H	-8.64165800	-3.49236900	1.68092500
H	10.19259100	-0.01474400	-2.42452800
H	9.54625800	1.61516300	-2.05994600
S	-8.23429500	3.33562100	-0.56427600

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***g*$^{+}$ Cys-S^{-}**
Ac-Ala-Cys-S^{-}-Ala$_9$-NHMe
optimized M11L/Def2SVP/H_2O

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C	-8.77765600	-0.63963400	2.35511300
H	-9.79196400	-0.99709700	2.11889100
C	-7.71809300	-1.20232800	1.47582800
O	-6.53794700	-1.12516500	1.74912200
N	-8.12093100	-1.76792400	0.33108000
H	-9.11005700	-1.86663700	0.13612200
C	-7.16511600	-2.29762000	-0.58675200
H	-6.48848200	-2.99683700	-0.04803200
C	-7.84793000	-3.02829800	-1.71130200
C	-6.23814300	-1.21331100	-1.12960300
H	-8.52686100	-2.36047700	-2.27269200
H	-7.10374100	-3.42546400	-2.42019900
H	-8.43812400	-3.88017100	-1.33134000
O	-5.09194900	-1.47537700	-1.43611300
N	-6.79024200	-0.02084600	-1.28796000
H	-7.70045700	0.19681000	-0.86560300
C	-6.05329100	1.14118300	-1.65859300
H	-5.59147600	1.00693700	-2.66048900
C	-7.02782900	2.32785500	-1.70012900
C	-4.88502100	1.39290200	-0.71292000
H	-6.41293700	3.24684500	-1.82303000
H	-7.59284600	2.23827600	-2.65547300
O	-3.73958200	1.52243600	-1.10005500
N	-5.23023100	1.45799900	0.56916000
H	-6.23373900	1.57152500	0.76546700
C	-4.25971700	1.71001300	1.57847700
H	-3.67088500	2.62523200	1.34066300
C	-4.93548300	1.87082400	2.91579500
C	-3.22473800	0.59355900	1.61585400
H	-5.51129900	0.96311400	3.17622000
H	-4.19857400	2.05888100	3.71367100
H	-5.63638000	2.72415300	2.89432100
O	-2.04935000	0.82451000	1.81403700
N	-3.69350300	-0.63804700	1.44235200
H	-4.70101100	-0.79767100	1.36395600
C	-2.79134900	-1.74422800	1.45880100
H	-2.17972300	-1.71739100	2.38764400
C	-3.54231500	-3.04656900	1.37629400
C	-1.77287400	-1.62894000	0.32750200
H	-4.12474400	-3.10768700	0.43830900
H	-2.84488500	-3.89981600	1.40463000
H	-4.24090200	-3.15288400	2.22460200
O	-0.59958600	-1.89323100	0.49555200
N	-2.26356900	-1.25327700	-0.84909200
H	-3.26639400	-1.09001600	-0.96828300
C	-1.38912300	-1.08779000	-1.96459600
H	-0.76482300	-1.99986900	-2.08889600
C	-2.17663000	-0.82872900	-3.22201000
C	-0.38110500	0.02649900	-1.70685200
H	-2.79959300	0.07873200	-3.11824400
H	-1.50237800	-0.69276200	-4.08338000
H	-2.84625300	-1.67752000	-3.44430500
O	0.78145300	-0.07982100	-2.03967000
N	-0.86043100	1.11824300	-1.11870800
H	-1.86020600	1.20283100	-0.91856700
C	0.01863800	2.20266000	-0.82180200
H	0.56409700	2.50741900	-1.74242400
C	-0.75109700	3.37274100	-0.26892600
C	1.11830600	1.76444800	0.14184000
H	-1.27067000	3.09517400	0.66705200
H	-0.07584300	4.21703900	-0.05374600
H	-1.50884600	3.72106100	-0.99259200
O	2.25982600	2.16101800	0.02730500
N	0.73265200	0.95083500	1.11983200
H	-0.25357800	0.70314800	1.22398500

C	1.68227500	0.46933500	2.06917900
H	2.27272400	1.32144700	2.47163800
C	0.98628800	-0.25457400	3.19140300
C	2.72256900	-0.42283500	1.39967100
H	0.40604200	-1.11392300	2.80685100
H	1.71627600	-0.62989200	3.92737800
H	0.28902700	0.41961900	3.71853400
O	3.89843100	-0.35364100	1.68982600
N	2.25517500	-1.28771900	0.50335800
H	1.25159300	-1.36020000	0.32385600
C	3.16149300	-2.14374900	-0.19176100
H	3.78743400	-2.70195900	0.53931300
C	2.40705000	-3.10985100	-1.06667700
C	4.16272900	-1.33050100	-1.00869200
H	1.78660400	-2.57022900	-1.80686100
H	3.10346700	-3.76705000	-1.61290500
H	1.73960700	-3.75082100	-0.46398200
O	5.32840300	-1.64489400	-1.09762100
N	3.65348300	-0.27031900	-1.63555500
H	2.65230900	-0.07393200	-1.58992900
C	4.50911900	0.56618200	-2.41162500
H	5.08977300	-0.05129800	-3.13115700
C	3.70715700	1.60325600	-3.15291100
C	5.57568300	1.21504900	-1.53059800
H	3.13942500	2.24275500	-2.45156900
H	4.36644800	2.25115600	-3.75410000
H	2.98618800	1.12384700	-3.83833800
O	6.73788600	1.28282800	-1.86715700
N	5.13363800	1.71563800	-0.37737900
H	4.13943800	1.67660100	-0.14454300
C	6.04607800	2.33909400	0.52565300
H	6.60486100	3.14567900	0.00113300
C	5.30877200	2.91601900	1.70574600
C	7.13733500	1.38074800	0.99801800
H	4.77232600	2.12294300	2.26016200
H	6.01034100	3.40904600	2.39862400
H	4.56818300	3.66828700	1.38167200
O	8.24942900	1.77165400	1.26259800
N	6.75341600	0.10922400	1.13549900
H	5.77104900	-0.13577500	1.01015700
C	7.65367800	-0.88462300	1.61396200
H	8.24348300	-0.46759200	2.46014700
C	6.89561100	-2.10177000	2.07656300
C	8.71365600	-1.29995000	0.59527000
H	6.29764000	-2.52248900	1.24608900
H	7.59243400	-2.87802800	2.43207900
H	6.20580400	-1.85074900	2.90107000
O	9.70172400	-1.89504200	0.96417700
N	8.43936500	-1.00071900	-0.67070900
H	7.56961900	-0.51421600	-0.87609700
C	9.29379600	-1.34145200	-1.74643900
H	8.83234400	-2.08296900	-2.42717700
H	-8.76388900	0.45942200	2.23949100
H	-8.54524700	-0.86390100	3.40762000
H	10.22083100	-1.77999100	-1.34405000
H	9.56115600	-0.45588400	-2.35257700
S	-8.15823000	2.43548200	-0.30641300

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***t* Cys-S$^-$**
Ac-Ala-Cys-S$^-$-Ala$_9$-NHMe
optimized M11L/Def2SVP/H_2O

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C	-8.92121000	-1.81150400	2.02018700
H	-9.94221800	-1.82683500	1.61082100
C	-7.85454900	-1.79140200	0.98480400
O	-6.67592100	-1.69989000	1.26807500
N	-8.24553300	-1.86384600	-0.29315100
H	-9.22271400	-2.02229900	-0.51089500
C	-7.27221300	-1.97206800	-1.33231200
H	-6.60238000	-2.83734100	-1.12841100
C	-7.93033400	-2.15860900	-2.67309000
C	-6.33094400	-0.77496300	-1.35265800
H	-8.60163500	-1.31579500	-2.91921500
H	-7.16971200	-2.22882600	-3.46690000
H	-8.52343200	-3.08933500	-2.69589600
O	-5.17101400	-0.90910200	-1.67836700
N	-6.86046100	0.40176500	-1.03494700
H	-7.85005100	0.45084100	-0.80990400
C	-6.08990900	1.60962300	-0.98554100
H	-5.61550500	1.81655400	-1.96932100
C	-6.99651100	2.77174900	-0.60424500
C	-4.93873700	1.46490800	0.00246400
H	-7.80616300	2.79188100	-1.37619800
H	-7.52573700	2.44965200	0.33188400
O	-3.79044000	1.74501200	-0.26129000
N	-5.28934400	0.99004400	1.20093400
H	-6.22950200	0.63538700	1.34610000
C	-4.30979000	0.79292500	2.21611500
H	-3.73160100	1.73262400	2.35042700
C	-4.95943500	0.40117500	3.51685200
C	-3.26762500	-0.23597200	1.79548700
H	-5.55705900	-0.52153700	3.39909600
H	-4.20005700	0.22137400	4.29517200
H	-5.62807600	1.20178000	3.87751100
O	-2.09408900	-0.09720900	2.07159300
N	-3.72816700	-1.30120600	1.14693500
H	-4.73051900	-1.40925100	0.98273800
C	-2.81538400	-2.30701900	0.70274200
H	-2.18813700	-2.64394100	1.55685900
C	-3.56193600	-3.47716900	0.11959400
C	-1.81705500	-1.73074900	-0.29840400
H	-4.17594500	-3.16364800	-0.74517800
H	-2.86253800	-4.25805400	-0.22093000
H	-4.23075400	-3.92966300	0.87285800
O	-0.63844600	-2.01878200	-0.26458600
N	-2.33368500	-0.91866200	-1.21412200
H	-3.34131000	-0.75067300	-1.24450600
C	-1.48973800	-0.30498500	-2.18658700
H	-0.87167300	-1.07914800	-2.69211400
C	-2.31262600	0.44280900	-3.20286400
C	-0.47310400	0.61782900	-1.52258600
H	-2.93047900	1.21846400	-2.71369900
H	-1.66362400	0.93226800	-3.94736200
H	-2.98883100	-0.24389700	-3.74096600
O	0.67800600	0.67374200	-1.90372400
N	-0.93833100	1.36803200	-0.52802900
H	-1.93222700	1.34698700	-0.28636900
C	-0.06098300	2.25545000	0.16477100
H	0.47124700	2.90394300	-0.56542700
C	-0.83186600	3.10389900	1.14183100
C	1.05382300	1.48403300	0.86577800
H	-1.33793100	2.47471600	1.89770800
H	-0.15974400	3.80149700	1.66769600
H	-1.60229900	3.70023200	0.62219600
O	2.19766200	1.88996400	0.87961400
N	0.68156200	0.36251100	1.47493600
H	-0.30398200	0.09145600	1.50409600

C	1.65274400	-0.44487300	2.13895400
H	2.24114000	0.17931600	2.84687600
C	0.98231100	-1.57166400	2.88050600
C	2.68525100	-0.97903500	1.15246800
H	0.40144900	-2.20912500	2.18778900
H	1.72879800	-2.20341700	3.38931100
H	0.29064400	-1.18169600	3.64759800
O	3.86428300	-1.03395700	1.43196500
N	2.20242300	-1.40571300	-0.01098600
H	1.19540500	-1.40812400	-0.18539400
C	3.09332800	-1.91459800	-1.00253500
H	3.73079500	-2.71256500	-0.56154900
C	2.32213600	-2.46207000	-2.17416000
C	4.08263900	-0.83904800	-1.44651300
H	1.69453200	-1.67696600	-2.63568700
H	3.00644200	-2.85436400	-2.94442800
H	1.65902800	-3.28633700	-1.85757200
O	5.25370200	-1.07987600	-1.63979100
N	3.55988600	0.37329400	-1.62531500
H	2.55704700	0.52990800	-1.51053100
C	4.40651300	1.45140000	-2.01868200
H	4.97754600	1.17018300	-2.93042900
C	3.59544600	2.69214200	-2.28506600
C	5.48335100	1.70864400	-0.96625200
H	3.03309500	3.00133500	-1.38403500
H	4.24771400	3.52768400	-2.58900000
H	2.86842000	2.51903600	-3.09812400
O	6.63929200	1.91692100	-1.26329000
N	5.05520700	1.70675600	0.29594600
H	4.06492500	1.56572800	0.50349900
C	5.97474800	1.93721700	1.36217400
H	6.52160500	2.89054500	1.18944700
C	5.24873200	1.99847700	2.68041900
C	7.07957000	0.88370700	1.41316100
H	4.72043200	1.04761900	2.88202400
H	5.95681100	2.18268500	3.50510200
H	4.50244600	2.81228300	2.68500900
O	8.19106600	1.15511300	1.80173400
N	6.70978800	-0.34495000	1.04365200
H	5.72760300	-0.53623600	0.84394700
C	7.62827200	-1.43183900	1.08627400
H	8.23331500	-1.36011400	2.01679700
C	6.89616300	-2.74865000	1.06019100
C	8.66805200	-1.40537300	-0.03256500
H	6.29147000	-2.83955000	0.13813200
H	7.61263700	-3.58567200	1.08907600
H	6.21670800	-2.84454100	1.92496500
O	9.67999100	-2.06265300	0.06931900
N	8.34921900	-0.66636100	-1.09080500
H	7.46223200	-0.16785200	-1.08322100
C	9.18173100	-0.54985300	-2.22943000
H	8.72088200	-0.99641900	-3.13195500
H	-8.80872300	-0.93156900	2.67403600
H	-8.78232700	-2.69799200	2.66083300
H	10.13004700	-1.07607800	-2.03584700
H	9.41015000	0.50705900	-2.46194300
S	-6.16084600	4.32579000	-0.41560100

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***g*⁻ Cys-SO_2^-**

Ac-Ala-Cys-SO_2^--Ala_9-NHMe

optimized M11L/Def2SVP/H_2O

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C	-8.45299800	-3.03820400	0.90157000
H	-9.49703100	-2.95727900	0.56364100
C	-7.46973600	-2.38331700	-0.00114900
O	-6.26981800	-2.43885800	0.20122300
N	-7.95635000	-1.70221300	-1.03936100
H	-8.95375700	-1.69836800	-1.21759400
C	-7.07668800	-1.08641100	-1.98230700
H	-6.46556000	-1.86094400	-2.49717800
C	-7.85851900	-0.29255100	-2.99575700
C	-6.06585000	-0.18758900	-1.28254400
H	-8.42049100	0.52824200	-2.51187200
H	-7.18157300	0.15488100	-3.74142900
H	-8.57404800	-0.93383500	-3.53940200
O	-4.90297200	-0.15803700	-1.62974100
N	-6.55544000	0.57368300	-0.31104800
H	-7.57261000	0.75147800	-0.22932900
C	-5.71534900	1.56180600	0.28787500
H	-5.23587400	2.18743700	-0.49836000
C	-6.54655000	2.45237900	1.17123600
C	-4.58095800	0.92877300	1.07296500
H	-6.97795900	1.90237800	2.03106000
H	-5.93470200	3.28571400	1.56414800
O	-3.50020600	1.46769300	1.19180900
N	-4.88092200	-0.22715000	1.66929900
H	-5.75031100	-0.69162200	1.41744800
C	-3.88794500	-0.96097300	2.38321000
H	-3.32339100	-0.25508200	3.02674900
C	-4.51812300	-2.03808200	3.22593500
C	-2.84070200	-1.53663600	1.43894800
H	-5.10656200	-2.73644900	2.60265500
H	-3.74841800	-2.62048900	3.75823400
H	-5.19189900	-1.59855300	3.98135200
O	-1.66412700	-1.55775200	1.73480500
N	-3.29758700	-2.02050400	0.28771500
H	-4.29857200	-2.01822500	0.08546100
C	-2.37617500	-2.50023200	-0.69186500
H	-1.68793700	-3.23638000	-0.22271000
C	-3.10658800	-3.14021500	-1.84197300
C	-1.45954600	-1.37197600	-1.16234800
H	-3.79773800	-2.42370000	-2.32338800
H	-2.39620500	-3.49915300	-2.60446400
H	-3.69512200	-4.00766500	-1.49563400
O	-0.27546100	-1.55106800	-1.35607700
N	-2.04783900	-0.19402800	-1.35071400
H	-3.06517100	-0.11083300	-1.28655500
C	-1.27251000	0.92936200	-1.76765600
H	-0.67424700	0.66254000	-2.66662500
C	-2.16335800	2.10456300	-2.07318800
C	-0.22821400	1.28933400	-0.71345900
H	-2.74501500	2.40756900	-1.18221000
H	-1.56698100	2.96996900	-2.40552700
H	-2.87553300	1.85685600	-2.87962000
O	0.90597800	1.59261400	-1.01925500
N	-0.65051900	1.26940700	0.54785400
H	-1.63763500	1.11263100	0.76183800
C	0.25835000	1.56822200	1.60763000
H	0.75035000	2.54789900	1.41803300
C	-0.46222500	1.60350000	2.92948800
C	1.40956100	0.56785000	1.63932400
H	-0.93457600	0.62788000	3.14986400
H	0.23753100	1.83966700	3.74773000
H	-1.25268200	2.37375900	2.92503600
O	2.54925300	0.92245300	1.85839500
N	1.07968400	-0.70525400	1.44449600
H	0.09958100	-0.97795400	1.34530200

C	2.09537700	-1.70945300	1.44991200
H	2.70336700	-1.62353200	2.37749100
C	1.48125800	-3.08166900	1.36165500
C	3.09377500	-1.48150200	0.31962400
H	0.88387300	-3.18906800	0.43704600
H	2.26253000	-3.85914600	1.36146900
H	0.81554500	-3.26978400	2.22193200
O	4.28508500	-1.64376200	0.47687200
N	2.56552300	-1.12472800	-0.84807600
H	1.55221300	-1.05952300	-0.96085500
C	3.42149800	-0.86774600	-1.96033500
H	4.09001600	-1.74045900	-2.13128300
C	2.60949300	-0.59210700	-3.19824800
C	4.37469900	0.28445600	-1.65162200
H	1.94977900	0.28358600	-3.05269800
H	3.26682300	-0.39289800	-4.06063200
H	1.97425800	-1.45947000	-3.45099100
O	5.54616400	0.25328700	-1.95624900
N	3.82176700	1.33123000	-1.03818100
H	2.82029200	1.34704100	-0.83802000
C	4.63546400	2.44987000	-0.69100700
H	5.17391700	2.82050800	-1.59054100
C	3.79608200	3.55353500	-0.10283000
C	5.74839400	2.03579700	0.26907900
H	3.27702900	3.21054800	0.81157000
H	4.42085400	4.42373700	0.15880100
H	3.03119600	3.89225400	-0.82384800
O	6.88664500	2.43652000	0.14935100
N	5.37548200	1.22652700	1.25917200
H	4.39924700	0.93950000	1.35154300
C	6.32842000	0.80133500	2.23172200
H	6.83190800	1.68776100	2.67776300
C	5.65288800	0.00333600	3.31590800
C	7.47219600	0.00024100	1.61507200
H	5.15693700	-0.89024200	2.89256000
H	6.38726500	-0.32956900	4.06782900
H	4.88738800	0.60756900	3.83396800
O	8.57716900	0.00841400	2.10356700
N	7.14252200	-0.72723400	0.54573800
H	6.16903400	-0.76429700	0.24357200
C	8.09436700	-1.54780700	-0.12318400
H	8.78489300	-1.97631300	0.63642200
C	7.40713000	-2.66637100	-0.86173900
C	9.02225900	-0.78968000	-1.07015500
H	6.69302600	-2.26402100	-1.60548300
H	8.14639700	-3.28682200	-1.39341300
H	6.84563100	-3.31388400	-0.16635600
O	9.98809100	-1.35309500	-1.53635300
N	8.68479400	0.46894100	-1.33136200
H	7.83282400	0.84396500	-0.92033300
C	9.43399700	1.30194100	-2.19679800
H	8.87590400	1.55550500	-3.11909100
H	-8.37098400	-2.59108000	1.90662500
H	-8.19051400	-4.10291200	1.00932700
H	10.35765000	0.77852100	-2.49080600
H	9.71280700	2.25264900	-1.70560100
S	-7.97295800	3.15978700	0.21819100
O	-7.31744600	3.49868000	-1.07896900
O	-8.83166600	1.91884600	0.08408200

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***g*⁺ Cys-SO_2^-**

Ac-Ala-Cys-SO_2^--Ala_9-NHMe

optimized M11L/Def2SVP/H_2O

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C	-8.51494700	-0.99742200	2.27220800
H	-9.47558400	-1.50914800	2.10120700
C	-7.41281900	-1.51177300	1.41912200
O	-6.24059900	-1.41392700	1.72267100
N	-7.77190900	-2.06170800	0.25143000
H	-8.75127100	-2.12069100	-0.00019600
C	-6.77490300	-2.47534700	-0.67940900
H	-6.07094100	-3.17218700	-0.17440300
C	-7.39387100	-3.16103000	-1.86724900
C	-5.90288500	-1.30419300	-1.11701200
H	-8.09578900	-2.49309600	-2.40005300
H	-6.61536500	-3.47025800	-2.58310500
H	-7.94691800	-4.06525000	-1.55925700
O	-4.72803100	-1.46570800	-1.38404500
N	-6.52167900	-0.14047500	-1.21589800
H	-7.53073700	-0.04450000	-1.02078200
C	-5.81541000	1.05501000	-1.55553800
H	-5.32143600	0.94503300	-2.54800400
C	-6.79038500	2.22130400	-1.61567200
C	-4.64582700	1.30497200	-0.59438100
H	-6.26311700	3.18462800	-1.47633800
H	-7.27859200	2.26677900	-2.60822600
O	-3.51661900	1.50647600	-0.99717300
N	-4.97726600	1.28395700	0.68681200
H	-5.98632600	1.31029600	0.91907000
C	-4.00054800	1.50886700	1.69544200
H	-3.43117200	2.44321400	1.48662600
C	-4.66504400	1.60622200	3.04452600
C	-2.93982200	0.41671100	1.68420600
H	-5.24345600	0.68896800	3.26298600
H	-3.92110300	1.74942700	3.84538400
H	-5.36271400	2.46143600	3.07270700
O	-1.76984700	0.66988700	1.89068100
N	-3.37507300	-0.81882600	1.45876300
H	-4.37664300	-1.00123800	1.35294800
C	-2.43587600	-1.89342800	1.40284400
H	-1.81466300	-1.89703600	2.32547800
C	-3.14276100	-3.21479000	1.25669100
C	-1.43418100	-1.68274900	0.27135400
H	-3.73428100	-3.24410800	0.32287500
H	-2.41614300	-4.04327600	1.23025700
H	-3.82670800	-3.39090200	2.10523600
O	-0.25461600	-1.93663000	0.41045500
N	-1.94486300	-1.24192000	-0.87261600
H	-2.95308100	-1.09744100	-0.96979400
C	-1.08925300	-1.00204400	-1.98840600
H	-0.45515600	-1.89660300	-2.17411800
C	-1.89564300	-0.67812700	-3.21851300
C	-0.09454500	0.11008000	-1.67742300
H	-2.52366100	0.21695000	-3.05490700
H	-1.23321000	-0.48832700	-4.07899000
H	-2.56150700	-1.51829800	-3.48144000
O	1.06495300	0.04445300	-2.03010700
N	-0.58718000	1.15541500	-1.01995700
H	-1.58580500	1.20189700	-0.80233000
C	0.27365400	2.23558000	-0.65812300
H	0.80305100	2.61493800	-1.56006300
C	-0.51453300	3.34692000	-0.01669800
C	1.38925300	1.75334100	0.26720200
H	-1.02188300	2.98951500	0.89869900
H	0.14553300	4.18610700	0.25775700
H	-1.28413900	3.73302200	-0.70813800
O	2.53110100	2.14812400	0.15408500
N	1.01465900	0.89938600	1.21526100
H	0.02952100	0.64952100	1.32568800

C	1.97950100	0.38409100	2.13033100
H	2.55714000	1.22263000	2.57817100
C	1.30576000	-0.41477500	3.21465900
C	3.03053900	-0.44914000	1.40475900
H	0.74061300	-1.26373500	2.78703000
H	2.04837600	-0.81482800	3.92451400
H	0.59839700	0.21433900	3.78267300
O	4.20512600	-0.38642700	1.70215900
N	2.57111100	-1.26157200	0.45691400
H	1.56696700	-1.33381800	0.27940800
C	3.47902900	-2.07232200	-0.28765300
H	4.12510700	-2.64778000	0.41152900
C	2.72698600	-3.01639300	-1.18844000
C	4.45548300	-1.21468800	-1.08795500
H	2.08929000	-2.45958200	-1.90066800
H	3.42624600	-3.64184800	-1.76733900
H	2.07682100	-3.68852400	-0.60132400
O	5.62529300	-1.51179000	-1.19945600
N	3.92897200	-0.14061500	-1.67177300
H	2.92559300	0.04380200	-1.61586500
C	4.76831400	0.73463500	-2.42230900
H	5.34199900	0.15393200	-3.17738900
C	3.94577200	1.79508300	-3.10540100
C	5.84426600	1.35398800	-1.53166700
H	3.37489300	2.39038500	-2.36829000
H	4.59007800	2.48118800	-3.67964900
H	3.22458100	1.34000100	-3.80705100
O	6.98984900	1.47990400	-1.90012100
N	5.42329500	1.76602300	-0.33452100
H	4.43725200	1.69181800	-0.08017900
C	6.34820300	2.34782500	0.58239500
H	6.90111600	3.17568900	0.08657200
C	5.62744400	2.87040100	1.79753900
C	7.44294200	1.36326100	0.99251600
H	5.09627100	2.05411100	2.32269700
H	6.33754700	3.33147300	2.50390700
H	4.88395500	3.63692600	1.51638400
O	8.57647600	1.72397300	1.20393100
N	7.03872900	0.09947800	1.14275400
H	6.04698700	-0.12881700	1.06449400
C	7.95084900	-0.90580400	1.57314500
H	8.55647700	-0.51933600	2.42234800
C	7.20547600	-2.14359700	1.99979500
C	8.98966000	-1.27138100	0.51274100
H	6.60129000	-2.54105500	1.16229400
H	7.90957300	-2.92836100	2.32174200
H	6.52265200	-1.92761200	2.84015400
O	10.06096600	-1.73195000	0.83724600
N	8.59283000	-1.09403300	-0.74491900
H	7.64445200	-0.76307700	-0.90918500
C	9.39667900	-1.42528300	-1.86167500
H	9.02839000	-2.32295800	-2.39712000
H	-8.64083600	0.07354300	2.02584100
H	-8.23862500	-1.07696400	3.33418700
H	10.42270500	-1.63421900	-1.51867900
H	9.43316300	-0.59514600	-2.59059100
S	-8.22322500	2.18331400	-0.43711000
O	-8.95437800	0.96083600	-0.92832400
O	-7.57396100	1.88723100	0.89086100

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***t* Cys-SO_2^-**

Ac-Ala-Cys-SO_2^--Ala_9-NHMe

optimized M11L/Def2SVP/H_2O

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C	-8.68446300	-2.84556700	1.45355200
H	-9.72148000	-2.71960400	1.10861400
C	-7.66070500	-2.45046200	0.45245900
O	-6.47027200	-2.44442400	0.70552200
N	-8.09360600	-2.07759700	-0.75685900
H	-9.07673200	-2.15857900	-0.98999600
C	-7.14676500	-1.82364200	-1.79532900
H	-6.49468300	-2.71485400	-1.93428300
C	-7.83741300	-1.49957000	-3.09259800
C	-6.17634700	-0.71780000	-1.40679400
H	-8.48224600	-0.60711100	-3.00079900
H	-7.09697200	-1.30203700	-3.88397600
H	-8.46418800	-2.34426200	-3.42695100
O	-5.01631200	-0.75967800	-1.75309600
N	-6.67406700	0.30602200	-0.71364100
H	-7.66352800	0.33254800	-0.48941700
C	-5.82473200	1.40631600	-0.36838300
H	-5.26792000	1.73449800	-1.27383900
C	-6.59403500	2.59652900	0.13013500
C	-4.75399700	0.98385600	0.62779600
H	-7.42463700	2.84749400	-0.56089700
H	-7.00643500	2.45020900	1.14916300
O	-3.64901000	1.48220100	0.61911000
N	-5.11425400	0.07266600	1.53150600
H	-5.99967500	-0.41448900	1.42727000
C	-4.14701300	-0.44651500	2.44639900
H	-3.61401400	0.40424700	2.92013700
C	-4.80070900	-1.29478900	3.50392900
C	-3.05782400	-1.21300300	1.70444400
H	-5.34818500	-2.14439500	3.05673700
H	-4.04552200	-1.69977700	4.19714600
H	-5.51570300	-0.69826400	4.09618800
O	-1.88868300	-1.11929900	2.01230200
N	-3.47441600	-1.99442600	0.70993100
H	-4.47061300	-2.08970900	0.50971400
C	-2.51777000	-2.70234500	-0.07887100
H	-1.84623700	-3.28621400	0.58771600
C	-3.20347400	-3.62590500	-1.05018500
C	-1.58404300	-1.72920400	-0.79528700
H	-3.86344600	-3.06539000	-1.73793500
H	-2.46387900	-4.17516200	-1.65519700
H	-3.81614900	-4.37099800	-0.51313200
O	-0.39354300	-1.94402400	-0.88760100
N	-2.16314000	-0.65379000	-1.32193400
H	-3.18084200	-0.56557200	-1.31442900
C	-1.37836000	0.32339900	-2.00586300
H	-0.76339400	-0.16910900	-2.79141100
C	-2.26245500	1.37053700	-2.63272500
C	-0.35496900	0.95623100	-1.06691100
H	-2.85942200	1.91126300	-1.87367500
H	-1.65680100	2.11021500	-3.18153100
H	-2.96155000	0.90877000	-3.35208100
O	0.78240500	1.18124200	-1.42477600
N	-0.80010800	1.26252400	0.14764800
H	-1.78893300	1.14772200	0.37728100
C	0.08140600	1.84100800	1.10904300
H	0.57869500	2.73739400	0.67683000
C	-0.67729300	2.22407100	2.35274800
C	1.23107900	0.89434100	1.43826900
H	-1.16164200	1.33994000	2.80806000
H	-0.00286100	2.67238800	3.10058200
H	-1.46398000	2.96226300	2.11949100
O	2.36250000	1.30336600	1.59803400
N	0.90594900	-0.38861900	1.56735600
H	-0.07021000	-0.68342200	1.50023700

C	1.91614100	-1.35574300	1.85503700
H	2.50860900	-1.02584300	2.73655000
C	1.29808100	-2.70233700	2.12419700
C	2.93615700	-1.43777300	0.72186000
H	0.71889600	-3.05319200	1.24982300
H	2.07581200	-3.45099700	2.34743700
H	0.61530900	-2.65501800	2.99059100
O	4.12398400	-1.55080400	0.93969100
N	2.43175000	-1.40411500	-0.50840300
H	1.42086100	-1.37672400	-0.65303000
C	3.30644300	-1.44283800	-1.63489400
H	3.98809500	-2.31797200	-1.55218800
C	2.51732100	-1.52598600	-2.91472800
C	4.24102400	-0.23492000	-1.64047800
H	1.83811200	-0.65925400	-3.01910900
H	3.19078100	-1.54465000	-3.78754700
H	1.90571800	-2.44510600	-2.94123600
O	5.41005900	-0.32859200	-1.94318400
N	3.67465100	0.92573500	-1.31176600
H	2.67117400	0.98024000	-1.12952400
C	4.47003000	2.10865500	-1.26840800
H	5.01424400	2.23489500	-2.22982000
C	3.61071500	3.31721000	-1.00508300
C	5.57868500	1.97961500	-0.22556500
H	3.07780700	3.22560700	-0.04036200
H	4.22359800	4.23345200	-0.97452900
H	2.85556000	3.44241200	-1.80120000
O	6.71479700	2.33837200	-0.44504000
N	5.20259500	1.46408900	0.94457100
H	4.22339300	1.22542300	1.11236100
C	6.15877800	1.29494700	1.98960300
H	6.67134000	2.26084800	2.19487800
C	5.48450400	0.80211500	3.24373200
C	7.29333500	0.35444700	1.58682100
H	4.98952600	-0.17152300	3.06709400
H	6.21826200	0.67579400	4.05696000
H	4.71718600	1.51801700	3.58782200
O	8.41515300	0.50025200	2.01104400
N	6.93871600	-0.64460700	0.77513300
H	5.95331300	-0.78090100	0.54845600
C	7.88991200	-1.61079100	0.33813900
H	8.53168300	-1.90657400	1.19720300
C	7.19179500	-2.82833500	-0.21114900
C	8.88308500	-1.07835600	-0.69300800
H	6.54985800	-2.55346000	-1.06940400
H	7.92830100	-3.57482900	-0.55071200
H	6.55281200	-3.29874100	0.55647300
O	9.92751700	-1.66244700	-0.88033700
N	8.49421700	0.00321300	-1.36123900
H	7.58094200	0.40163600	-1.15612900
C	9.28188500	0.61183300	-2.36735500
H	8.84902300	0.48152300	-3.37889500
H	-8.53616300	-2.25826400	2.37413700
H	-8.52832000	-3.90238500	1.72688500
H	10.28397700	0.15414400	-2.36706900
H	9.39127100	1.69782000	-2.19132800
S	-5.59018400	4.15506200	0.10159000
O	-5.22045900	4.18023700	-1.34946900
O	-6.66950200	5.13854400	0.41666400

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***g*⁻ Cys-SO_3^-**

Ac-Ala-Cys-SO_3^--Ala_9-NHMe

optimized M11L/Def2SVP/H2O

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C	-8.23232700	-3.24398200	1.16384200
H	-9.28053400	-3.16542100	0.83899700
C	-7.25675900	-2.64126400	0.21817000
O	-6.06005100	-2.62827800	0.44340800
N	-7.74553800	-2.09119600	-0.89602600
H	-8.73723600	-2.15125300	-1.09603200
C	-6.86399000	-1.57102200	-1.89207800
H	-6.21753400	-2.38260400	-2.29407700
C	-7.64595700	-0.93560400	-3.01203600
C	-5.89858000	-0.56029300	-1.29546800
H	-8.25332000	-0.08674100	-2.64513000
H	-6.96647000	-0.55441600	-3.79107000
H	-8.32197000	-1.66644200	-3.48878900
O	-4.73372600	-0.52145800	-1.62720200
N	-6.42787300	0.30100500	-0.43035300
H	-7.44549800	0.40414600	-0.34292800
C	-5.62585300	1.37921300	0.04853200
H	-5.15011800	1.91438200	-0.80319000
C	-6.47068100	2.36117100	0.82679400
C	-4.47473800	0.86641300	0.90402200
H	-6.85045300	1.92417200	1.77097100
H	-5.87308900	3.25319200	1.08440200
O	-3.40055200	1.42580400	0.93151000
N	-4.75626500	-0.20338000	1.64591000
H	-5.62864400	-0.69970500	1.48028400
C	-3.75139200	-0.82178600	2.44992300
H	-3.21108500	-0.03252300	3.01337100
C	-4.36200000	-1.81077400	3.40648300
C	-2.67738700	-1.47120900	1.58422300
H	-4.92855700	-2.59160400	2.86643000
H	-3.58116000	-2.30637800	4.00584200
H	-5.05166300	-1.30413200	4.10309900
O	-1.50222700	-1.40332000	1.87686000
N	-3.11166000	-2.11299600	0.50314900
H	-4.11116800	-2.17291600	0.30323300
C	-2.17012000	-2.68228100	-0.40763100
H	-1.47557100	-3.35172100	0.14508700
C	-2.87747500	-3.45476500	-1.48897100
C	-1.26659500	-1.60027300	-0.99587900
H	-3.56673300	-2.80298000	-2.05707400
H	-2.15288900	-3.89059000	-2.19609700
H	-3.46395300	-4.28440300	-1.05697800
O	-0.07750900	-1.78059600	-1.15306400
N	-1.87369600	-0.46693200	-1.33873400
H	-2.89121600	-0.38995400	-1.27938900
C	-1.11632500	0.60649900	-1.89909800
H	-0.50250500	0.23033600	-2.74671800
C	-2.02984800	1.70655900	-2.37237900
C	-0.09536600	1.13475600	-0.89762900
H	-2.63762800	2.10534500	-1.53866500
H	-1.44807300	2.53888400	-2.80091900
H	-2.71695700	1.33729500	-3.15363400
O	1.03009100	1.43598600	-1.23604700
N	-0.52860600	1.26640400	0.35317000
H	-1.50982900	1.09433000	0.58082500
C	0.35445800	1.74800000	1.36521900
H	0.82552400	2.69972700	1.03386500
C	-0.38922000	1.96284500	2.65686900
C	1.52790400	0.79182800	1.56510600
H	-0.84912600	1.02029300	3.00893300
H	0.29132600	2.32839500	3.44314100
H	-1.19241300	2.70939100	2.52860500
O	2.65310200	1.19721800	1.76888100
N	1.22329200	-0.50167900	1.53314000
H	0.25221900	-0.80154700	1.42912700

C	2.24653500	-1.48249600	1.69708700
H	2.83977400	-1.25863400	2.61078400
C	1.64511300	-2.85947600	1.79797800
C	3.25936400	-1.40419300	0.55718400
H	1.05461400	-3.09982600	0.89394000
H	2.43247100	-3.62306800	1.90926400
H	0.97487900	-2.93245300	2.67209400
O	4.45264400	-1.49351600	0.75434200
N	2.74125500	-1.25491100	-0.65883700
H	1.72848800	-1.24179800	-0.79318300
C	3.60434100	-1.13815000	-1.78961200
H	4.29872900	-2.00670400	-1.82834800
C	2.80054100	-1.06692500	-3.06099200
C	4.51930500	0.07610400	-1.65022000
H	2.11485600	-0.19901400	-3.04671900
H	3.46312900	-0.96963500	-3.93669300
H	2.19340400	-1.97908300	-3.19559200
O	5.69290300	0.03402500	-1.94687500
N	3.93282400	1.18727400	-1.20569200
H	2.92775900	1.21354300	-1.02527200
C	4.71481900	2.36898100	-1.03907300
H	5.23830000	2.61474100	-1.98908700
C	3.84623400	3.52490600	-0.61883500
C	5.84431700	2.13717800	-0.03815500
H	3.32946200	3.30601900	0.33423800
H	4.44934000	4.43786700	-0.48364000
H	3.07817000	3.73771000	-1.38317700
O	6.96843000	2.54625100	-0.22887100
N	5.49644800	1.48042200	1.06881500
H	4.52922100	1.18510900	1.21107200
C	6.46855700	1.22430100	2.08004800
H	6.97094500	2.17470400	2.36642600
C	5.82101800	0.60691600	3.29198100
C	7.60836500	0.33915100	1.57742200
H	5.33934600	-0.35493900	3.03403400
H	6.56993000	0.41799000	4.07880800
H	5.04825600	1.27464400	3.71220700
O	8.73124600	0.44951500	2.00971200
N	7.25616000	-0.57734000	0.67310700
H	6.27305400	-0.69123700	0.42600300
C	8.20856100	-1.49248300	0.14174800
H	8.87083400	-1.84571300	0.96247900
C	7.51102400	-2.67004000	-0.48825400
C	9.17185700	-0.86590500	-0.86480000
H	6.83708600	-2.33209100	-1.29824600
H	8.24568800	-3.37126200	-0.91659600
H	6.90385500	-3.21575000	0.25484000
O	10.20724600	-1.42955300	-1.14260900
N	8.76726500	0.27877800	-1.40659500
H	7.85523300	0.64326600	-1.14239200
C	9.51628000	0.97487100	-2.38536000
H	9.09128200	0.86586800	-3.40328300
H	-8.12582900	-2.76156600	2.14948700
H	-7.98099400	-4.30784000	1.30624900
H	10.54425800	0.57895200	-2.40673800
H	9.56129800	2.05508000	-2.15818900
S	-7.89989500	2.91244100	-0.09919600
O	-8.48573700	3.96883200	0.69632900
O	-7.37845100	3.33048700	-1.38629300
O	-8.74882600	1.71894300	-0.18226400

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***g*⁺ Cys-SO_3^-**

Ac-Ala-Cys-SO_3^--Ala_9-NHMe

optimized M11L/Def2SVP/H2O

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C	8.44694200	1.24962800	2.18484100
H	9.37620600	1.81392000	2.00776200
C	7.30863000	1.70994000	1.34768300
O	6.14684400	1.55648400	1.66690300
N	7.62331600	2.26279100	0.16729800
H	8.59337300	2.41344600	-0.08244900
C	6.58887300	2.63451700	-0.74012200
H	5.87431800	3.31511200	-0.22732900
C	7.14938900	3.32194100	-1.95591100
C	5.74547100	1.42987300	-1.13519700
H	7.85823500	2.67129400	-2.50018400
H	6.34017900	3.59515600	-2.65191700
H	7.67843700	4.24946400	-1.67692900
O	4.56757200	1.54885400	-1.39902000
N	6.39398600	0.27541300	-1.20174200
H	7.39901200	0.23234500	-1.00464100
C	5.71858600	-0.94867800	-1.48972800
H	5.23049400	-0.89882000	-2.48778700
C	6.71426600	-2.10391500	-1.51019700
C	4.54600700	-1.18561300	-0.52648600
H	6.19988500	-3.06804900	-1.34592100
H	7.20767100	-2.17097100	-2.49755800
O	3.42886200	-1.42974100	-0.93232900
N	4.85274600	-1.09985800	0.76078300
H	5.84314300	-1.08131700	1.02454200
C	3.86595800	-1.31808000	1.76306000
H	3.31438500	-2.26376800	1.56176600
C	4.51453100	-1.37990700	3.12136100
C	2.79470500	-0.23871000	1.71652200
H	5.07676700	-0.45060200	3.32995000
H	3.76109700	-1.51571100	3.91428100
H	5.22095900	-2.22642000	3.17717500
O	1.62755400	-0.49771300	1.92666900
N	3.21840200	0.99470700	1.45860700
H	4.21725500	1.18075500	1.33915300
C	2.26505000	2.05497800	1.36863600
H	1.64341200	2.07685800	2.29045200
C	2.95485800	3.37997000	1.18264100
C	1.26604200	1.79406800	0.24415600
H	3.54068000	3.39272800	0.24481600
H	2.21907700	4.19934200	1.13763100
H	3.64064400	3.58732300	2.02272300
O	0.08316900	2.03330000	0.37547800
N	1.78457800	1.32577900	-0.88584400
H	2.79485300	1.20057500	-0.97943500
C	0.93791300	1.04425600	-1.99857700
H	0.29129900	1.92359100	-2.21102000
C	1.75599000	0.69956900	-3.21526200
C	-0.04015000	-0.07569200	-1.66405700
H	2.40098400	-0.17770200	-3.02260200
H	1.10124100	0.46988300	-4.07190600
H	2.40604100	1.54431100	-3.50206600
O	-1.19843800	-0.03910600	-2.02307800
N	0.46737000	-1.09735100	-0.98009500
H	1.46503300	-1.12299900	-0.75803200
C	-0.37580600	-2.18440700	-0.59790000
H	-0.89328700	-2.59431800	-1.49325900
C	0.42871800	-3.26641000	0.07268200
C	-1.50479300	-1.70173200	0.31077600
H	0.92646000	-2.87994700	0.98161800
H	-0.21806000	-4.10967300	0.36554600
H	1.20716000	-3.65623900	-0.60661200
O	-2.63867300	-2.11878300	0.19914000
N	-1.14970900	-0.82429400	1.24452500
H	-0.16968500	-0.55589700	1.35412900

C	-2.12674300	-0.30413100	2.14479100
H	-2.69253700	-1.14170900	2.60906500
C	-1.46941500	0.52773300	3.21447600
C	-3.18680900	0.49964500	1.39847200
H	-0.91363300	1.37525500	2.77158500
H	-2.22179400	0.93322700	3.91082000
H	-0.75669600	-0.07827900	3.80065300
O	-4.36219000	0.42647200	1.68906100
N	-2.73211900	1.30196400	0.43934800
H	-1.72809500	1.38819600	0.26866000
C	-3.64703700	2.08638100	-0.32422500
H	-4.30025200	2.67138700	0.36029300
C	-2.90379000	3.01678800	-1.24609400
C	-4.61414100	1.19822300	-1.10320900
H	-2.26103600	2.45095600	-1.94663400
H	-3.60869400	3.62323300	-1.83827300
H	-2.25951700	3.70736300	-0.67409200
O	-5.79091800	1.46499000	-1.20755600
N	-4.06970100	0.12515500	-1.67617400
H	-3.06304500	-0.04071500	-1.62669900
C	-4.90113300	-0.77981600	-2.39912300
H	-5.49200700	-0.22640600	-3.16140600
C	-4.06799900	-1.84250000	-3.06581700
C	-5.95777100	-1.39535100	-1.48382600
H	-3.48213700	-2.41346400	-2.32117600
H	-4.70541300	-2.55057300	-3.62073900
H	-3.35933800	-1.39152200	-3.78268200
O	-7.11251400	-1.52321300	-1.82788000
N	-5.51689500	-1.80079900	-0.29322400
H	-4.52727300	-1.72144800	-0.05307500
C	-6.42296600	-2.39096400	0.63786600
H	-6.94767600	-3.24986800	0.16400500
C	-5.68405400	-2.85944900	1.86433800
C	-7.55048800	-1.43704100	1.02729000
H	-5.18115900	-2.01216600	2.36752400
H	-6.37808600	-3.32722900	2.58202100
H	-4.91434100	-3.60622100	1.60127700
O	-8.66018400	-1.83977700	1.28422000
N	-7.20069800	-0.15100600	1.10507900
H	-6.22180300	0.11318800	0.99193800
C	-8.14035900	0.84219800	1.50299600
H	-8.73112600	0.46323900	2.36626400
C	-7.43004200	2.11213600	1.89449700
C	-9.19531700	1.15228200	0.44277900
H	-6.83566300	2.50138200	1.04621700
H	-8.15829600	2.88412500	2.19153400
H	-6.74363400	1.93960700	2.74175000
O	-10.22445100	1.70755600	0.75794100
N	-8.87353200	0.81145700	-0.80127700
H	-7.96937400	0.37525400	-0.96665600
C	-9.72222300	1.04938800	-1.90873300
H	-9.36873300	1.88609400	-2.54386800
H	8.63541300	0.18959500	1.93218200
H	8.17843800	1.30425900	3.25009700
H	-10.73028100	1.30549800	-1.54499500
H	-9.79754900	0.15421700	-2.55200200
S	8.07692300	-2.02369000	-0.34472000
O	8.76998000	-3.27888700	-0.49694900
O	8.85368700	-0.86116000	-0.77193300
O	7.48566500	-1.82871700	0.97766300

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Ac-Ala-Cys-SO_3^--Ala_9-NHMe

optimized M11L/Def2SVP/H2O

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C	-8.50320000	-2.79298300	1.83736100
H	-9.52007400	-2.85906700	1.42267100
C	-7.44489700	-2.57820600	0.81617400
O	-6.27248300	-2.45078400	1.11249100
N	-7.83416000	-2.50811000	-0.46284200
H	-8.79841200	-2.70308300	-0.70741800
C	-6.85430400	-2.42745100	-1.49819200
H	-6.12397500	-3.25955200	-1.38549200
C	-7.49323500	-2.50732300	-2.85899400
C	-6.00458800	-1.17353500	-1.37189600
H	-8.21057200	-1.68329700	-3.02499700
H	-6.72595100	-2.45314300	-3.64734700
H	-8.03179500	-3.46252600	-2.98271000
O	-4.84310800	-1.16957800	-1.71200500
N	-6.60832300	-0.07992700	-0.90859600
H	-7.59866600	-0.10684400	-0.68819300
C	-5.87436500	1.14272800	-0.78171000
H	-5.38165300	1.39179100	-1.74561400
C	-6.82465300	2.25647500	-0.41561300
C	-4.72208700	0.96304700	0.21035900
H	-7.58091500	2.36977100	-1.21575100
H	-7.36632800	2.03862800	0.52604700
O	-3.60331100	1.35806600	-0.02056900
N	-5.03674500	0.32487400	1.33780800
H	-5.95073300	-0.10532900	1.43717900
C	-4.03422800	0.06273600	2.31794300
H	-3.49768900	1.01022900	2.54016000
C	-4.64487400	-0.48630800	3.57949300
C	-2.95182500	-0.86615500	1.77987700
H	-5.20813900	-1.41637900	3.37865500
H	-3.86293400	-0.71320300	4.32202500
H	-5.33613800	0.24575000	4.03123800
O	-1.78548900	-0.71344600	2.07728700
N	-3.36007300	-1.85373800	0.98787300
H	-4.35592100	-2.00632500	0.82039300
C	-2.39124500	-2.73670200	0.42054600
H	-1.74455500	-3.14823200	1.22618500
C	-3.06264700	-3.85795700	-0.32563700
C	-1.42731000	-1.96698600	-0.48098200
H	-3.67729900	-3.46943800	-1.15847500
H	-2.31519900	-4.55018400	-0.74633300
H	-3.71725200	-4.43879400	0.34781800
O	-0.23690900	-2.20327000	-0.48674700
N	-1.98532700	-1.05353100	-1.26920900
H	-2.99869900	-0.92690000	-1.26930100
C	-1.17811800	-0.26622700	-2.14447600
H	-0.51237600	-0.93382700	-2.73408000
C	-2.03860500	0.54899400	-3.07361800
C	-0.22007700	0.62376100	-1.36066500
H	-2.69727400	1.23615700	-2.51054100
H	-1.41424500	1.15124100	-3.75387700
H	-2.67483800	-0.10719400	-3.69278400
O	0.91898500	0.81206200	-1.73482800
N	-0.71637500	1.18867500	-0.26474200
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