Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Pt(IV) Complex Selectively Oxidizes alpha-Synuclein Methionine Disclosed by NMR

Bin-Bin Pan,[a] Hui-Zhong Liu,[a] Wei-Han Meng,[a] and Xun-Cheng Su*[a]

a. State Key Laboratory of Elemento-organic Chemistry, Research Center for Analytical Sciences, College of Chemistry, Nankai University, Tianjin 300071, China.

E-mail: xunchengsu@nankai.edu.cn

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Experimental procedures

Protein expression and purification. Mutants (M1G, M1G/M5I, M116I/M127I, M5I/M116I/M127I (*3I*), M1G/M5I/M116I/M127 (*4M*)) were prepared by site-directed mutagenesis using wild type alpha-synuclein (αS) as the template. The proteins were expressed and purified as previously described.[1, 2] For the M1G/M5I and *4M* mutants, site-directed mutagenesis inserted a glycine codon between the first amino acid and the second amino acid codon. The mass spectrometry indicated that the first methionine was cleaved by methionine aminopeptidase [3] in *E. coli* to obtain the corresponding mutant.

***cis,cis,trans*-$[Pt(NH_3)_2Cl_2Br_2]$ synthesis**. The *cis,cis,trans*-$[Pt(NH_3)_2Cl_2Br_2]$ was synthesized as previously reported [4]. The purity of this compound was determined by UV spectrophotometer.

ESI-Q-TOF Measurements: 100 µM ^{14}N αS in 20 mM 2-(N-morpholino) ethanesulfonic acid (MES) buffer pH 6.4 was incubated with Pt(IV) complex at 298K. The reaction mixture was extracted at different incubation time for mass spectrometry. All samples were analyzed on an Agilent 1290 series HPLC system equipped with a 6545 series LC-ESI-QTOF (Agilent). The protein sample was injected into a C8 column (Agilent ZORBAX 300SB-C8 column, 2.1 × 150 mm) and run through by gradient elution at a column temperature of 70°C. Buffer A of the mobile phases consists of double distilled water containing 0.1% formic acid, and buffer B consists 100% acetonitrile containing 0.1% formic acid. The linear gradient conditions were as following: buffer A of 95% in 0-2 min, 95-40% in 2-10 min, 40-20% in 10-11 min, 20-10% in 11-12 min, 10% in 12-14 min, 10-95% in 14-14.5 min, 95% in 14.5-16.5 min. The mobile-phase flow rate was 0.5 mL/min. The column effluent was continuously characterized by capillary ESI source of the Agilent 6545 Q-TOF mass spectrometer and ESI mass spectra were acquired in positive electrospray ionization (ESI) mode using the m/z range 600−2,000 in profile mode. The raw data were converted to zero charge mass spectra using maximum entropy deconvolution algorithm over the region 6.4–7.1 min with BioConfirm Software (Agilent Technologies Inc., V10.0). The deconvolution settings: mass range, 600.0-2000.0 Dalton; mass step, 1.0000 Dalton; baseline factor, 7.00; adduct, proton; isotope width, automatic.[5]

NMR Measurements. All NMR experiments were performed on a Bruker Avance 600 MHz or 800 MHz NMR spectrometer equipped with a QCI-cryoprobe. Unless noted otherwise, NMR spectra were recorded in 20 mM MES buffer, pH 6.4, and at 298 K. The 20 mM stock solution of Pt(IV) was made by dissolving the compound in N, N-dimethylformamide-d7 (DMF-d7). 2D ^{1}H-^{15}N-HSQC spectra were measured on 100 µM ^{15}N protein in the absence and presence of Pt(IV) complex in 20 mM MES buffer (pH 6.5) at 298K. The cross-peak intensity ratio was determined by I/I_0, in which I_0 and I are the cross-

peak intensities recorded in the absence and presence of Pt(IV), respectively. Then the ratio were normalized.

Preparation of ^{15}N-methionine-selective labeled αS: *E.coil* was grown in LB medium at first, the cells were transferred into M9 medium at OD_{600} 0.7-0.8, and added 20 kinds of amino acid (2 g/L of non-labeled ^{14}N amino acid and 80 μg/mL ^{15}N labeled methionine) and 0.2% glucose and 0.01% $^{14}N\ NH_4Cl$ after incubation of 30 min, then the protein over-expression was induced by adding a final concentration of 1 mM IPTG. After 5 h IPTG induction, the cells were harvested.[6] 2D ^{1}H-^{15}N HSQC spectra were measured after mixing 150 μM ^{15}N labeled methionine αS with the Pt(IV) at different incubation duration time and at 298K.

MALDI-TOF measurements. The sample matrix was prepared with saturated α-cyno-4-hydroxycinnamic acid in water: CH3CN (1:1) and 00.1% CF_3COOH. The samples were analyzed on Bruker matrix-assisted laser desorption / ionization time of flight mass spectrometry(MALDI-TOF).

Preparation of oxidized αS: 200 μL 100 μM ^{14}N protein in 20 mM MES pH 6.4 were treated with 4% H_2O_2 at 4°C for 30 min, then followed by a PD-10 column to remove excess of H_2O_2, and the flow-through fractions were collected and concentrated using a Millipore concentrator with a 3k MWCO. The oxidized αS samples were incubated at room temperature in the presence of 1 equivalent of cisplatin for 72 h, then aliquots (1 μL) were diluted for mass spectrometry.

For the αS_Pt sample preparation, 100 μM ^{14}N αS in 20 mM MES pH 6.4 were incubated with 1 equivalent of cisplatin at 25°C for about 20 h, then treated with 4% H_2O_2 at 4°C for 30 min.

Fluorescence assay. The degree of αS aggregation was measured by using the Thioflavin T (ThT) fluorescence assay.[7] A round-bottom 96-well polypropylene dish was used to incubate all samples. Each well contains 100 μM protein sample in 20 mM MES buffer (pH 6.5), 100 mM NaCl, 0.05% NaN_3, and 20 μM ThT to a final volume of 200 μL. Protein samples were incubated in the absence and presence of 100 μM Pt(IV) at 37°C under constant shaking. The fluorescence was measured every about 12 h. Each emission spectrum was recorded with an excitation wavelength of 446 nm.

H_2O_2 oxidate αS. 0.3 mM αS (^{14}N / ^{15}N labeled methionines) incubated with different concentrations of H_2O_2 in 20 mM MES at pH 6.4 and 298 K. After the addition of H_2O_2, the mixture was incubated at 298 K for 25 minutes, then mass spectrometry (ESI-Q-TOF) and NMR (800 MHz NMR spectrometer) were collected, respectively.

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Figure

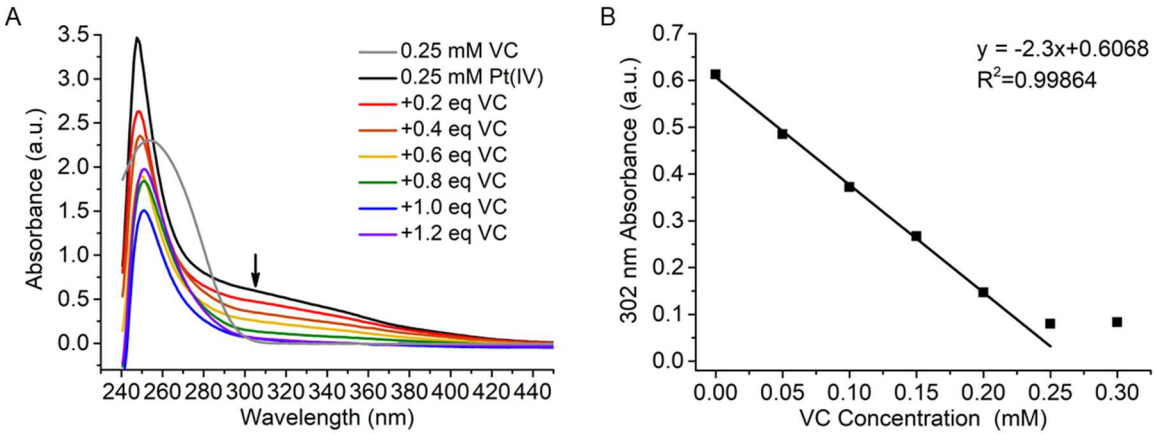


Figure S1. Characterization of the purity of *cis,cis,trans*-$[Pt(NH_3)_2Cl_2Br_2]$ (Pt(IV)) compounds. (A) UV absorption curve of Pt(IV) at 240 nm-400 nm recorded for 0.25 mM Pt(IV) was gradually titrated with different concentrations of ascorbic acid (VC). (B) Function curve of the concentration of VC and the UV absorption value at 302 nm, the VC concentration-UV absorbance was fitted by four data points from 0 to 0.2 mM.

Pt(IV) was able to be reduced by ascorbic acid quantitatively, and its purity was detected by monitoring the change in absorbance at 302 nm by UV spectrum. The UV absorption value of Pt(IV) mixed with an equal amount of VC is substituted into the fitting formula, the total concentration of Pt(IV) in the solution is about 0.229 mM, and the purity is about 91.6%

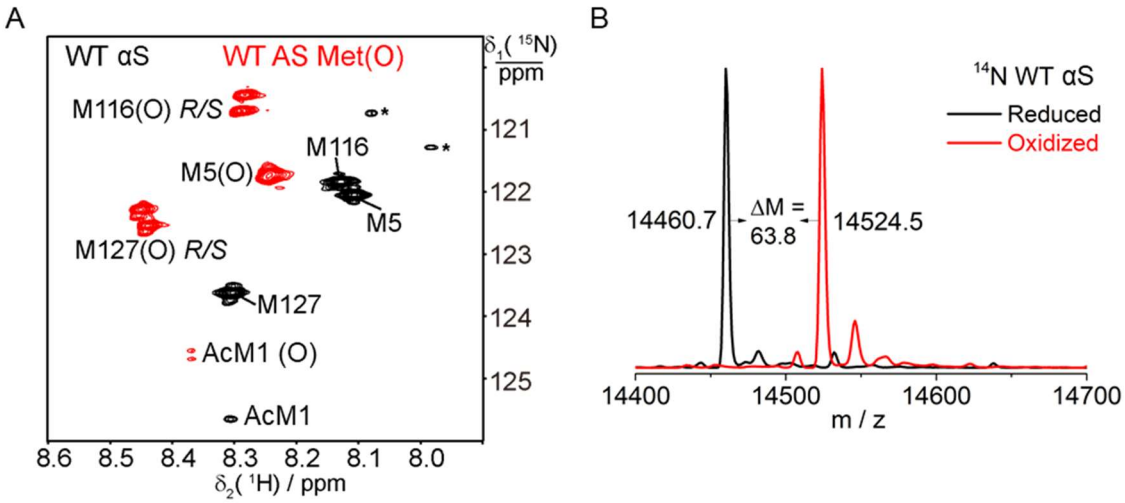


Figure S2. (A) Overlay of the ^{1}H-^{15}N HSQC spectra recorded for ^{15}N-methionine enriched αS (black) and 4% H_2O_2 treated αS (red), in which the label of AcM1 denotes the acetylated M1. (B) Mass spectrum recorded for αS (Reduced) (black) and after treatment with 4% H_2O_2 (Oxidized) (red).

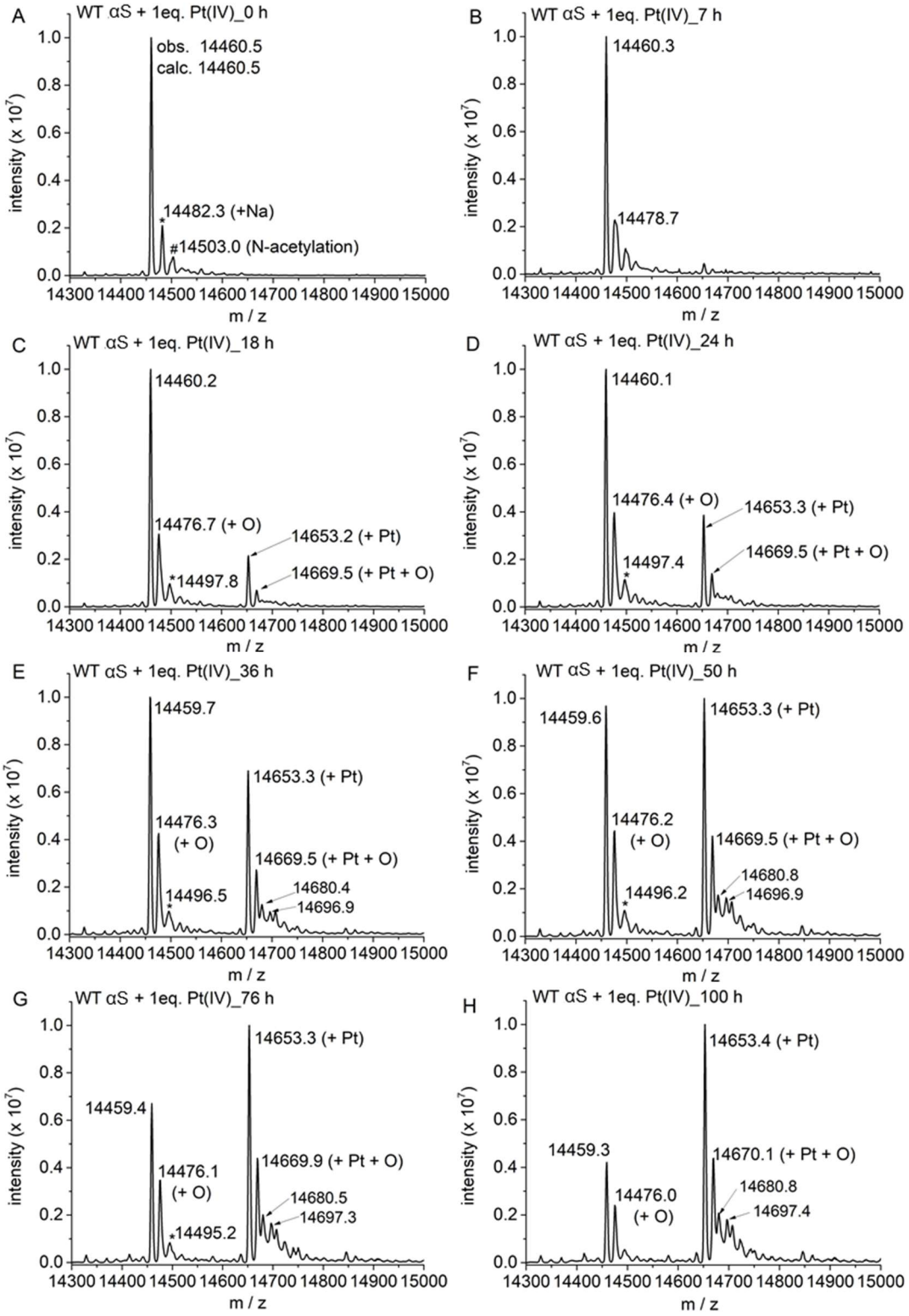


Figure S3. Mass spectra recorded for the mixture of αS after incubation with one equivalent of Pt(IV) for different time at 25°C. The peak plus one Na ion is marked with an asterisk (*). The acetylated protein (measured molecular mass as 14503.0 Dalton) was marked with #. The labels in parentheses represent the corresponding atoms added to αS after incubation with Pt(IV). All spectra are displayed as deconvoluted MS.

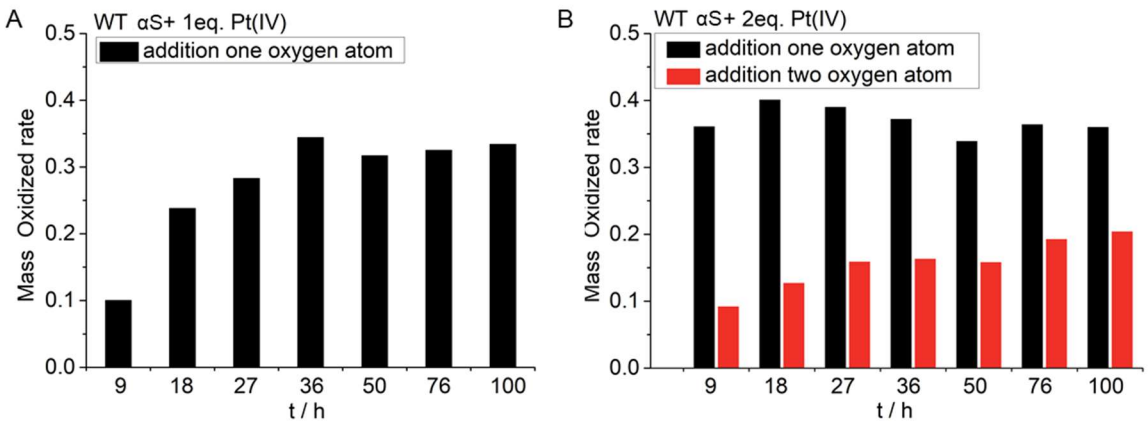


Figure S4. The fractions of oxygen added to αS after αS incubated with Pt(IV) determined by ESI-Q-TOF spectra. (A) The increase fraction of oxidized methionine was recorded for αS incubated with one equivalent of Pt(IV) at 25°C for different time. (B) The increase fraction of the oxidized methionine was recorded for αS incubated with two equivalents of Pt(IV) at 25°C for different time. Quantification of the oxidation extent was obtained by the peak–height ratios in the mass spectrum between the oxidized, non-oxidized, and coordinated with Pt forms of each αS molecule.

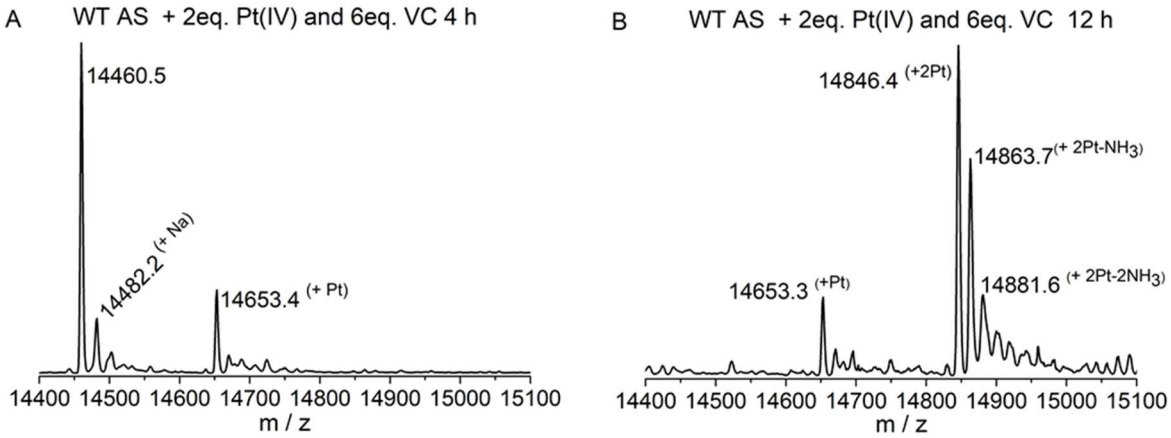
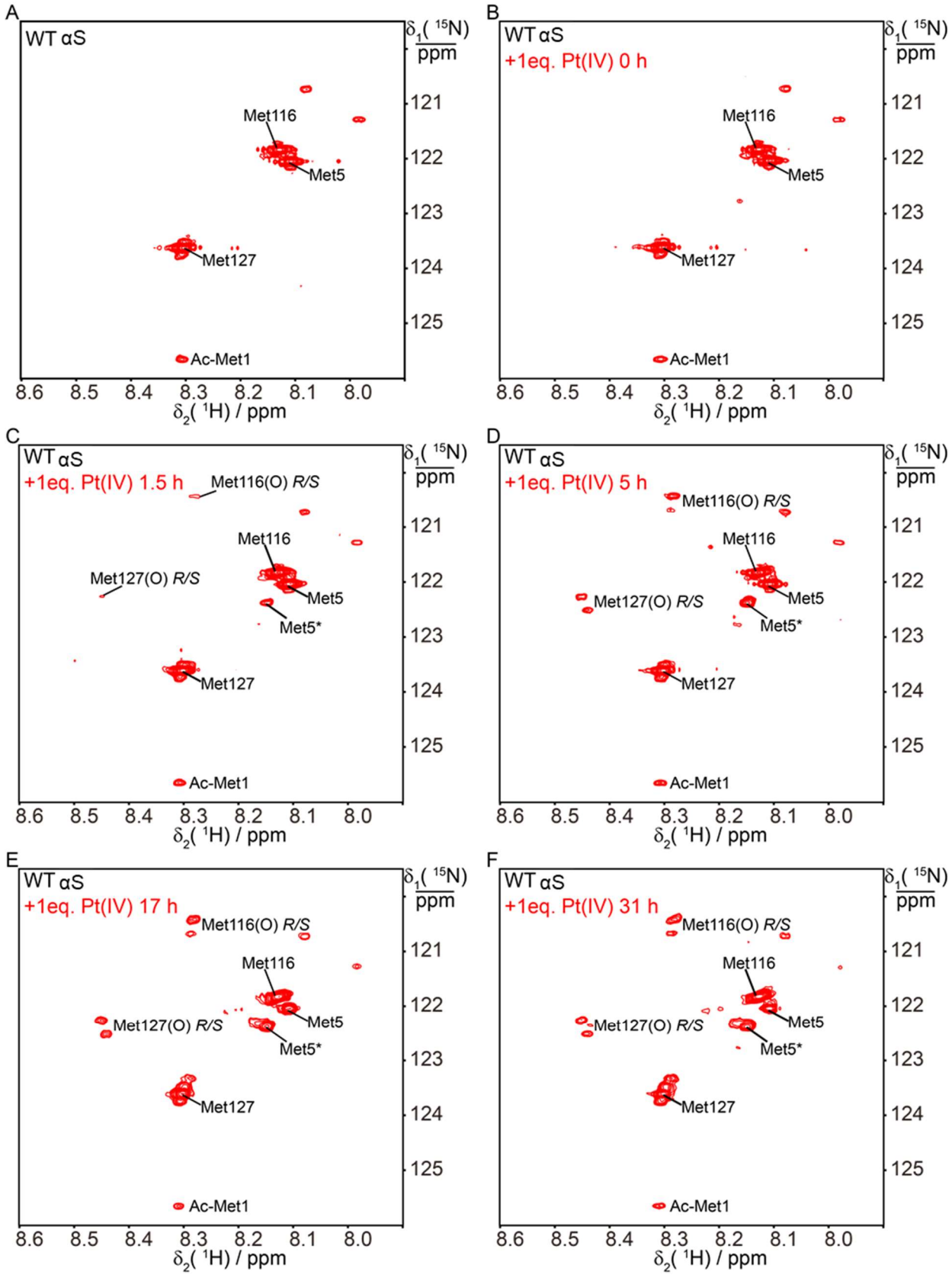


Figure S5. The products of 0.1 mM αS incubated with 0.2 mM Pt(IV) and 0.6 mM VC for 4 h (A) and 12 h (B) were characterized by the ESI-Q-TOF.


A
WT αS
Met116
Met5
Met127
Ac-Met1
B
WT αS
+1eq. Pt(IV) 0 h
Met116
Met5
Met127
Ac-Met1
C
WT αS
+1eq. Pt(IV) 1.5 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
Ac-Met1
D
WT αS
+1eq. Pt(IV) 5 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
Ac-Met1
E
WT αS
+1eq. Pt(IV) 17 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
Ac-Met1
F
WT αS
+1eq. Pt(IV) 31 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
Ac-Met1
δ1(15N) ppm
121
122
123
124
125
8.6 8.5 8.4 8.3 8.2 8.1 8.0
δ2(1H) / ppm

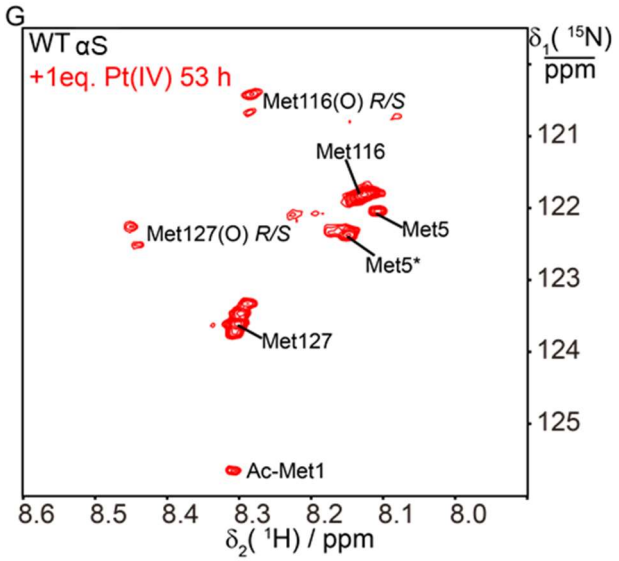


Figure S6. ^{1}H-^{15}N HSQC spectra recorded for 0.15 mM ^{15}N-Met enriched αS after incubation with 1 equivalent Pt(IV) from 0 h to 53 h in 20 mM MES at pH 6.4 and 298 K. The oxidized M116 and M127 were labeled as Met116(O) and Met127(O), respectively. The new cross-peak (8.12, 122.57 ppm) corresponding to the chemical shift of M5 was labeled with Met5* due to the N-terminal conformational change caused by the oxidation of M116 or M127 or both M116 and M127.

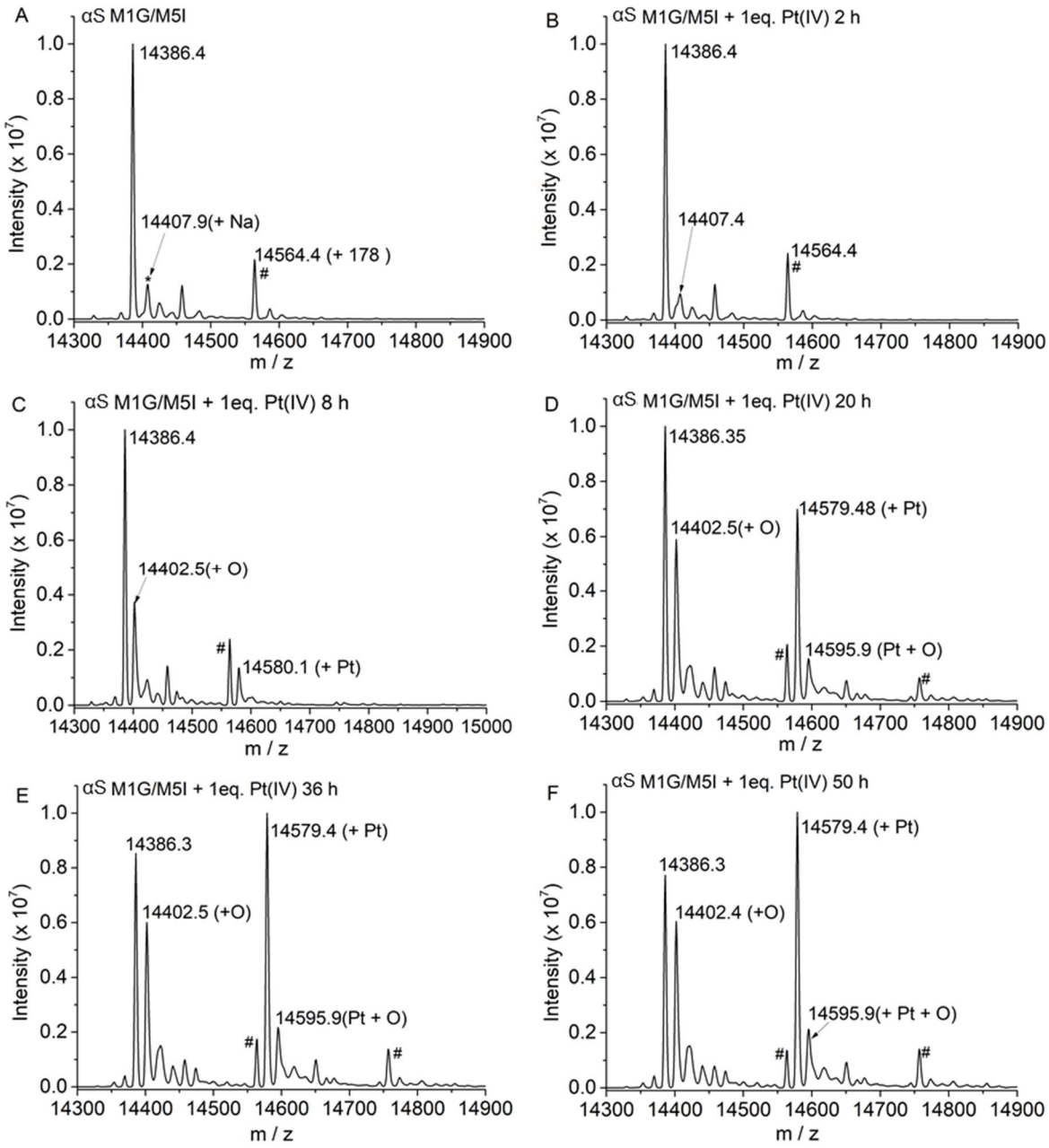


Figure S7. Mass spectra recorded for the mixture of αS M1G/M5I after incubation with one equivalent of Pt(IV) for different time at 25°C. The mass weight of some mutants expressed in *E. coli* with an increase of 178 Dalton, that is the post-translational modification of gluconoylation[8] at the N-terminus glycine, were marked with #.

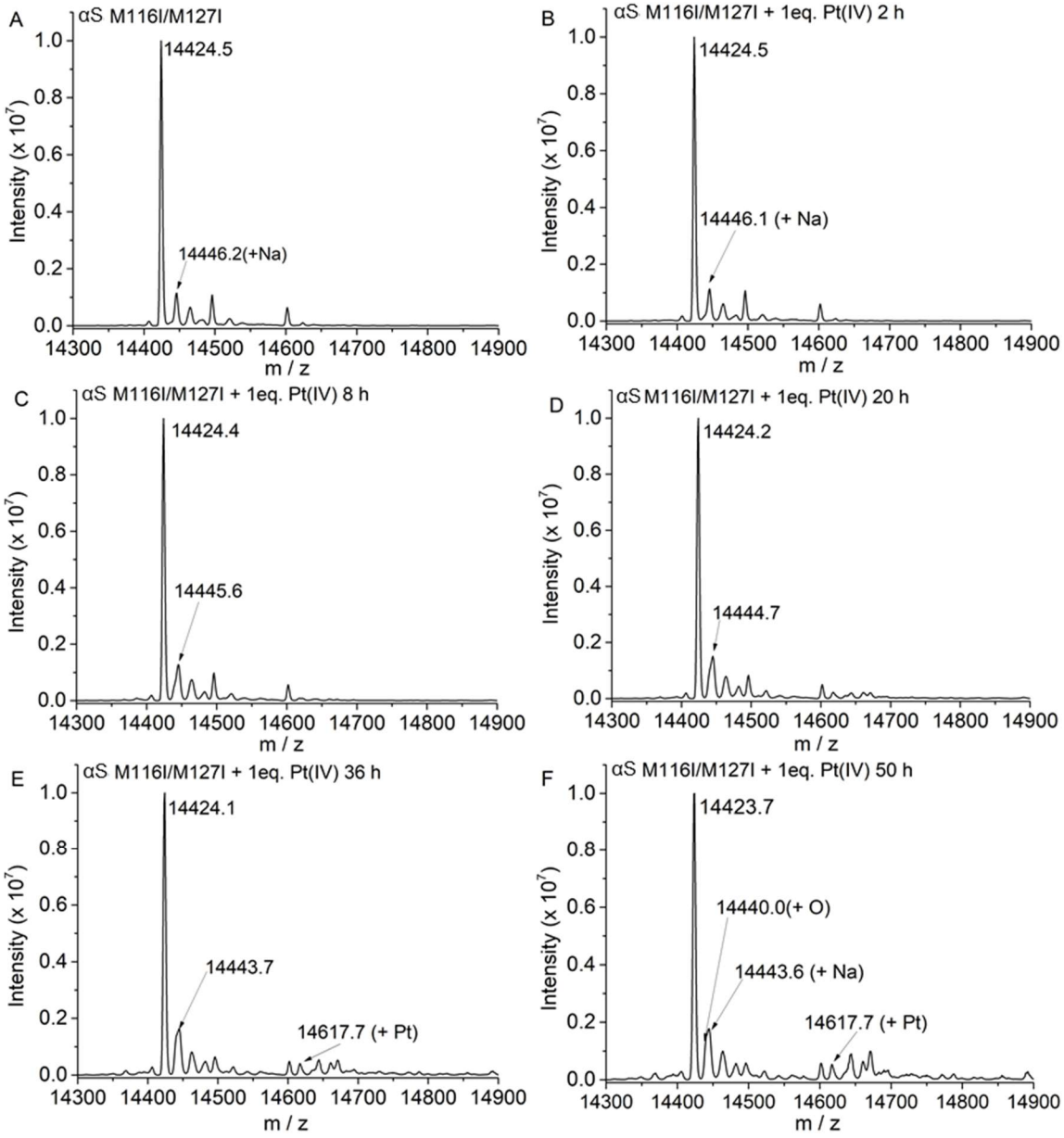
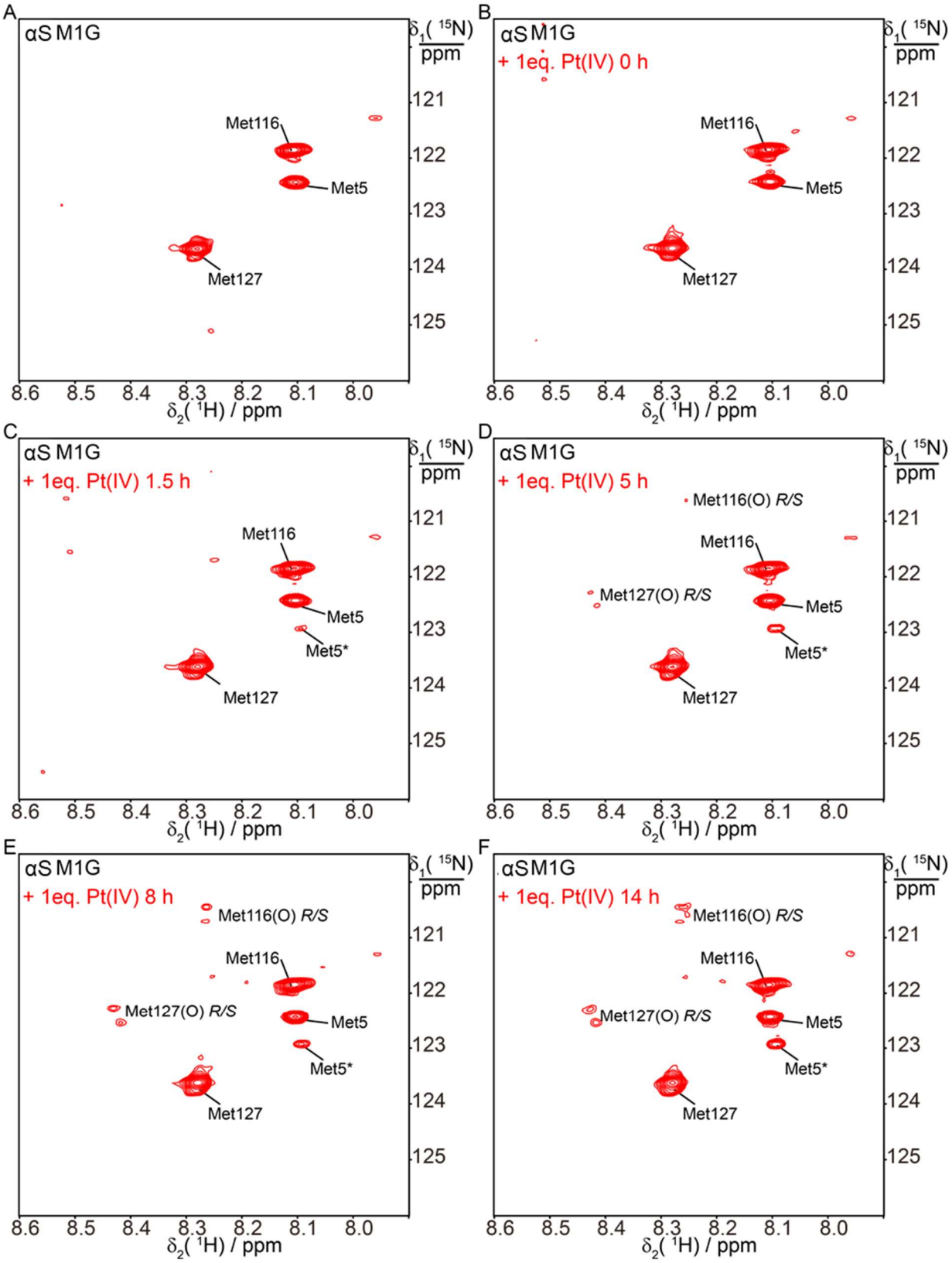


Figure S8. Mass spectra recorded the mixture of αS M116I/M127I after incubation with one equivalent of Pt(IV) for different time at 25°C.


A
αS M1G
Met116
Met5
Met127
B
αS M1G
+ 1eq. Pt(IV) 0 h
Met116
Met5
Met127
C
αS M1G
+ 1eq. Pt(IV) 1.5 h
Met116
Met5
Met5*
Met127
D
αS M1G
+ 1eq. Pt(IV) 5 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
E
αS M1G
+ 1eq. Pt(IV) 8 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
F
αS M1G
+ 1eq. Pt(IV) 14 h
Met116(O) R/S
Met116
Met127(O) R/S
Met5
Met5*
Met127
δ1(15N) ppm
121
122
123
124
125
8.6 8.5 8.4 8.3 8.2 8.1 8.0
δ2(1H) / ppm

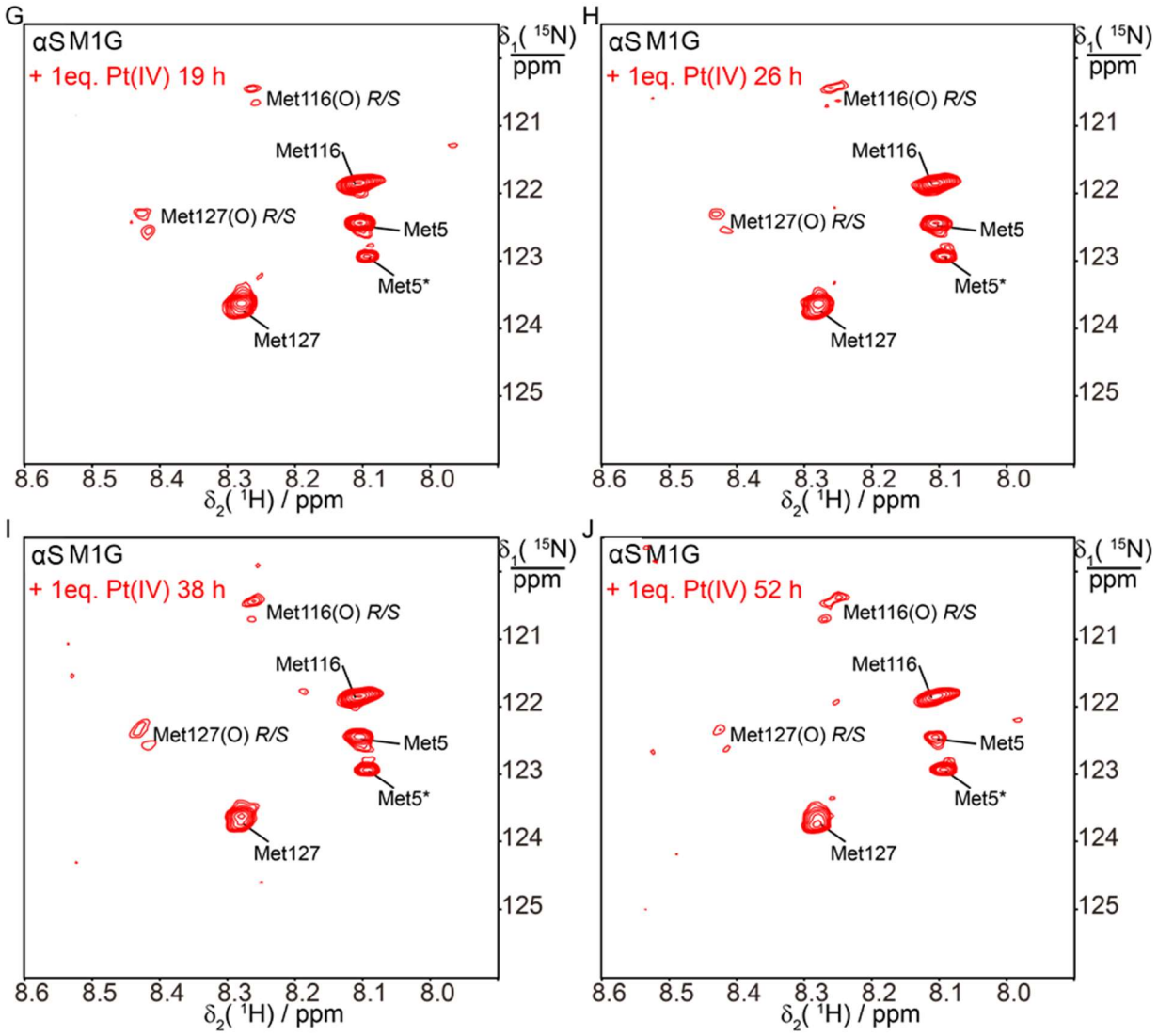


Figure S9. ^{1}H-^{15}N HSQC spectra recorded for 0.15 mM ^{15}N-Met enriched αS M1G after incubation with 0.15 mM Pt(IV) from 0 h to 52 h in 20 mM MES at pH 6.4 and 298 K.

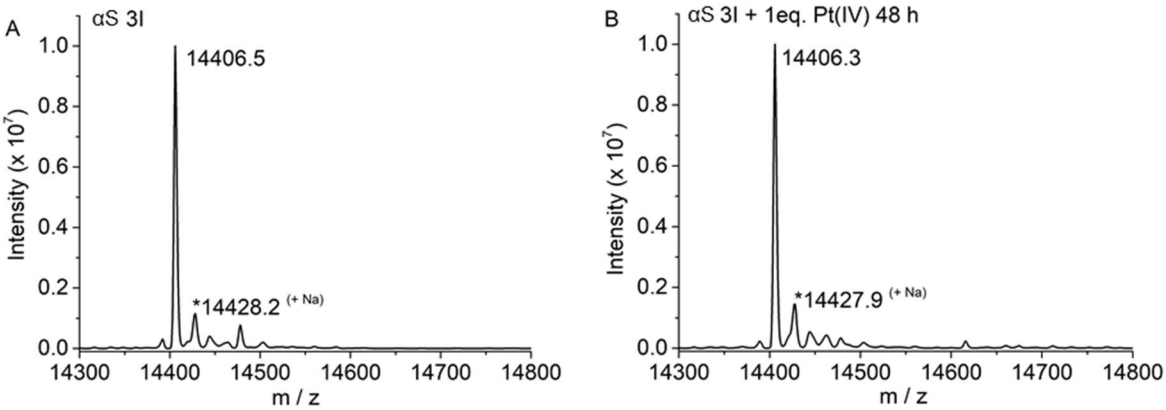


Figure S10. (A) Mass spectrum recorded for 0.1 mM M5I/M116I/M127I (3I). (B) Mass spectrum recorded for the mixture of 3I after incubation with one equivalent of Pt(IV) at 25°C for 48 h.

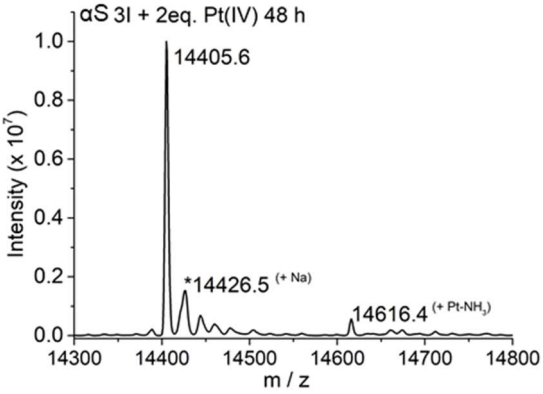


Figure S11. Mass spectrum recorded for the mixture of 3I after incubation with two equivalents of Pt(IV) at 25°C for 48 h.

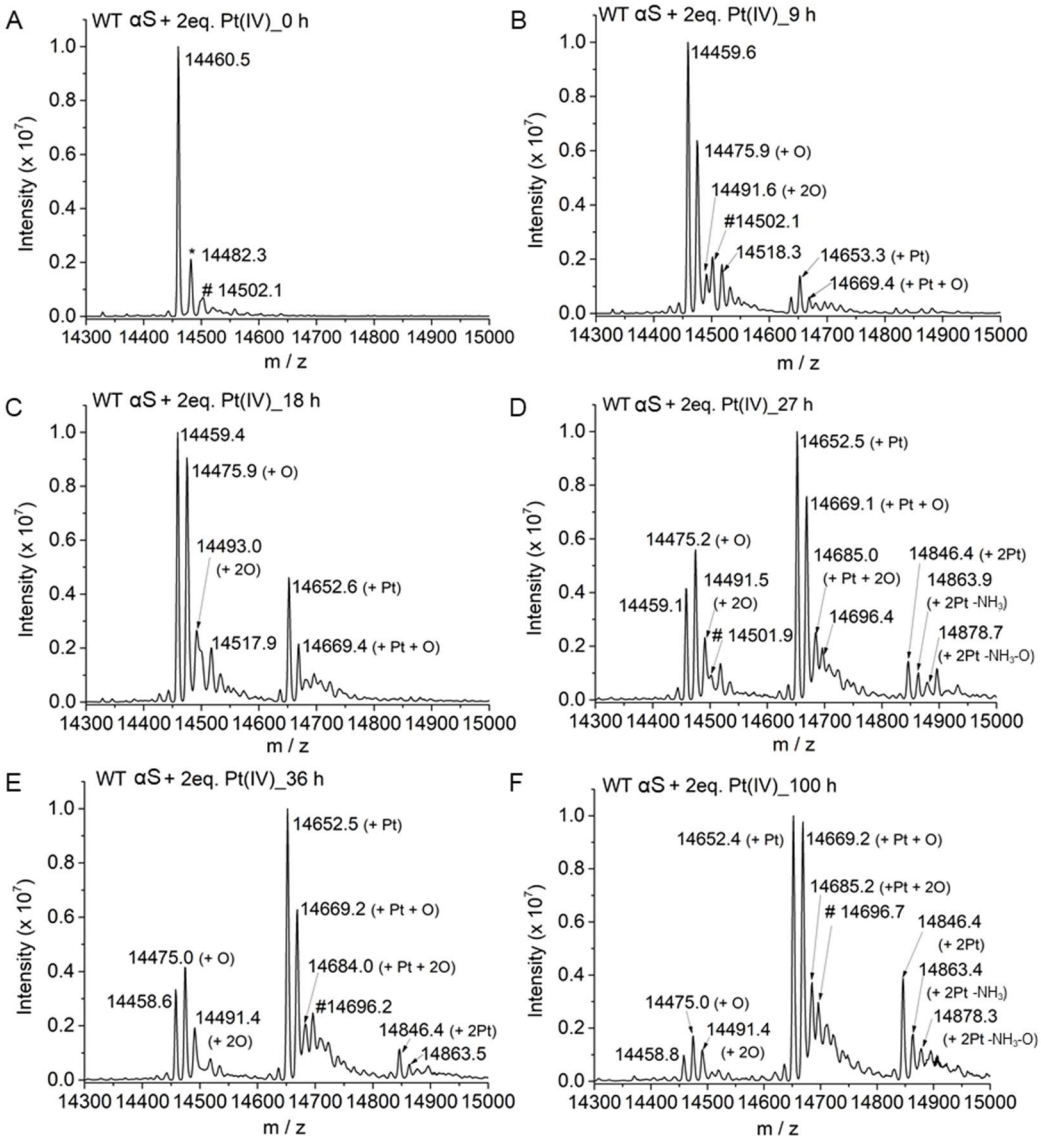


Figure S12. The products of 0.1 mM αS incubated with 0.2 mM Pt(IV) for different time were characterized by ESI-Q-TOF. The peak of N-terminal acetylated αS was marked with #, and the peak with addition one Na^+ was marked with an asterisk.

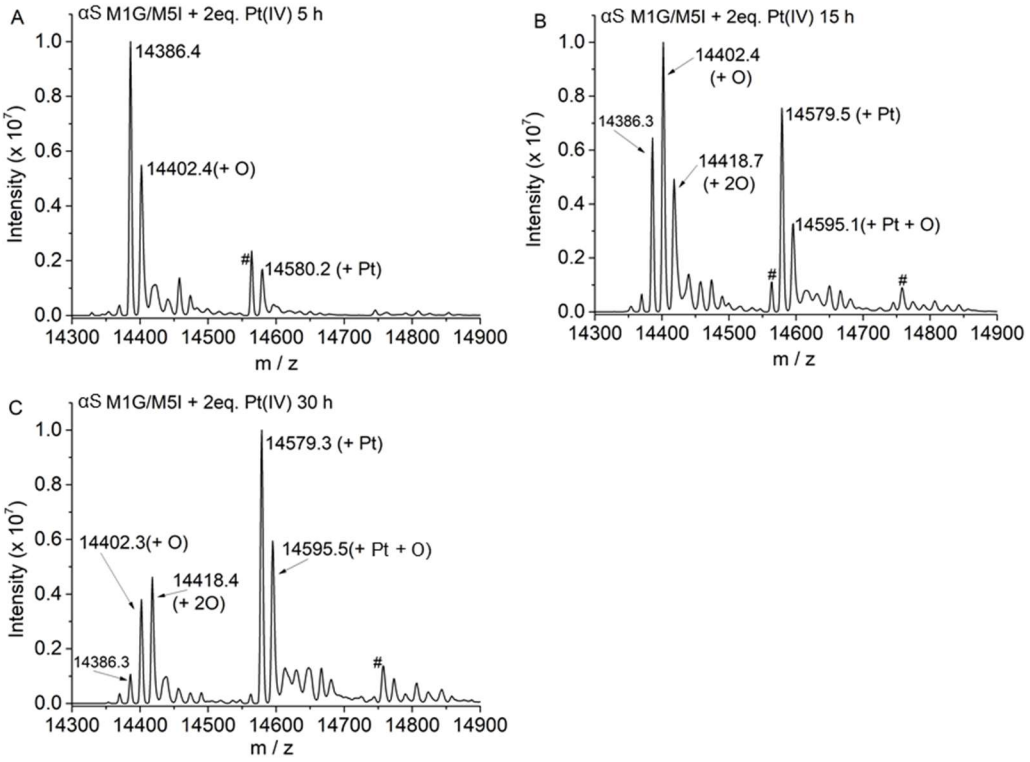


Figure S13. The products of 0.1 mM αS M1G/M5I after incubation with 0.2 mM Pt(IV) for different time at 25°C were characterized by ESI-Q-TOF. The gluconoylation [8] modified αS was marked with #.

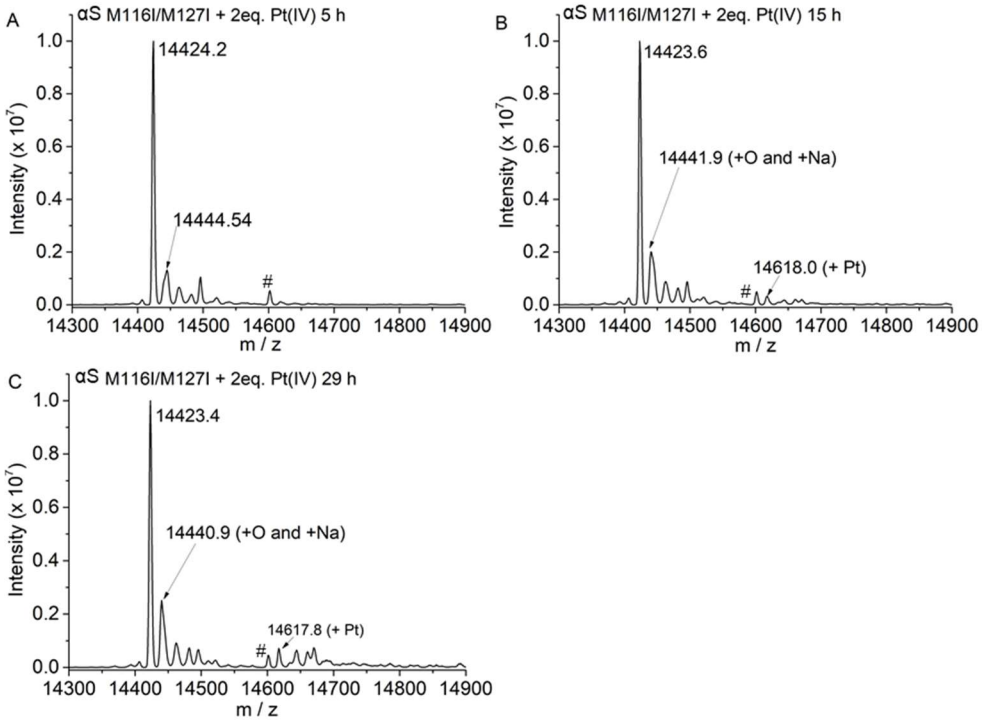


Figure S14. The products of 0.1 mM αS M116I/M127I after incubation with 0.2 mM Pt(IV) for different time at 25°C were characterized by ESI-Q-TOF. The gluconoylation[8] modified αS was marked with #.

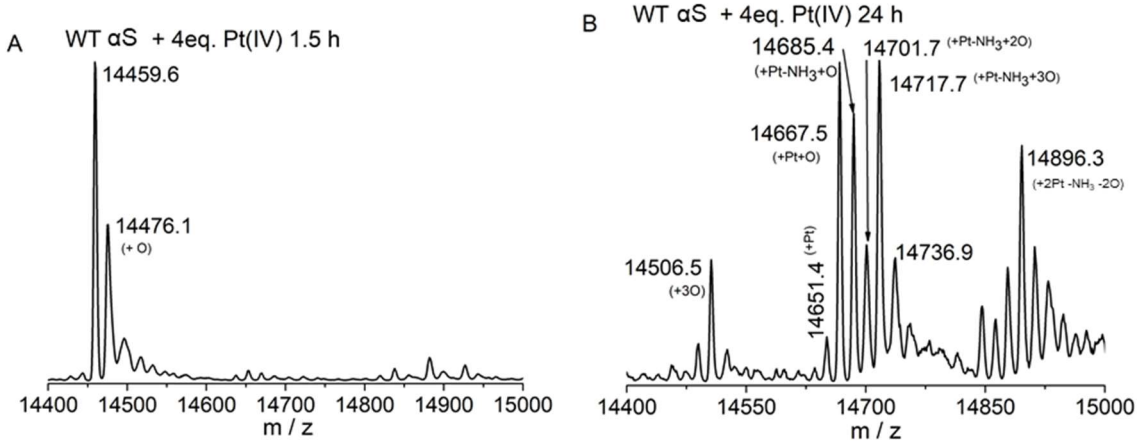


Figure S15. The products of 0.1 mM αS after incubation with 0.4 mM Pt(IV) for different time at 25°C were characterized by ESI-Q-TOF.

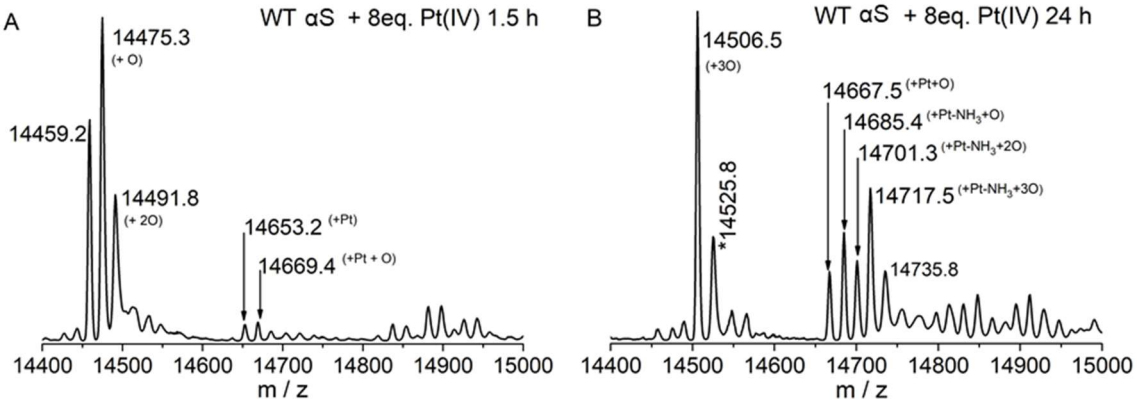


Figure S16. The products of 0.1 mM αS after incubation with 0.8 mM Pt(IV) for different time at 25°C were characterized by ESI-Q-TOF.

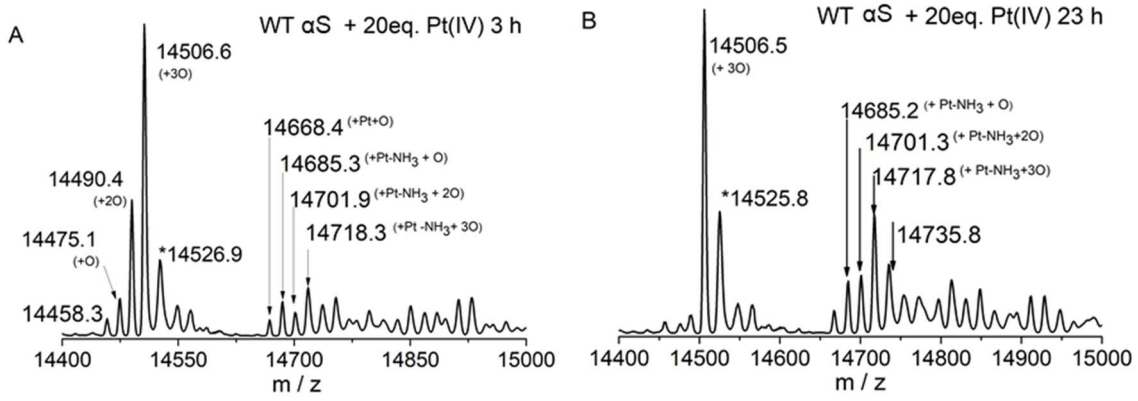
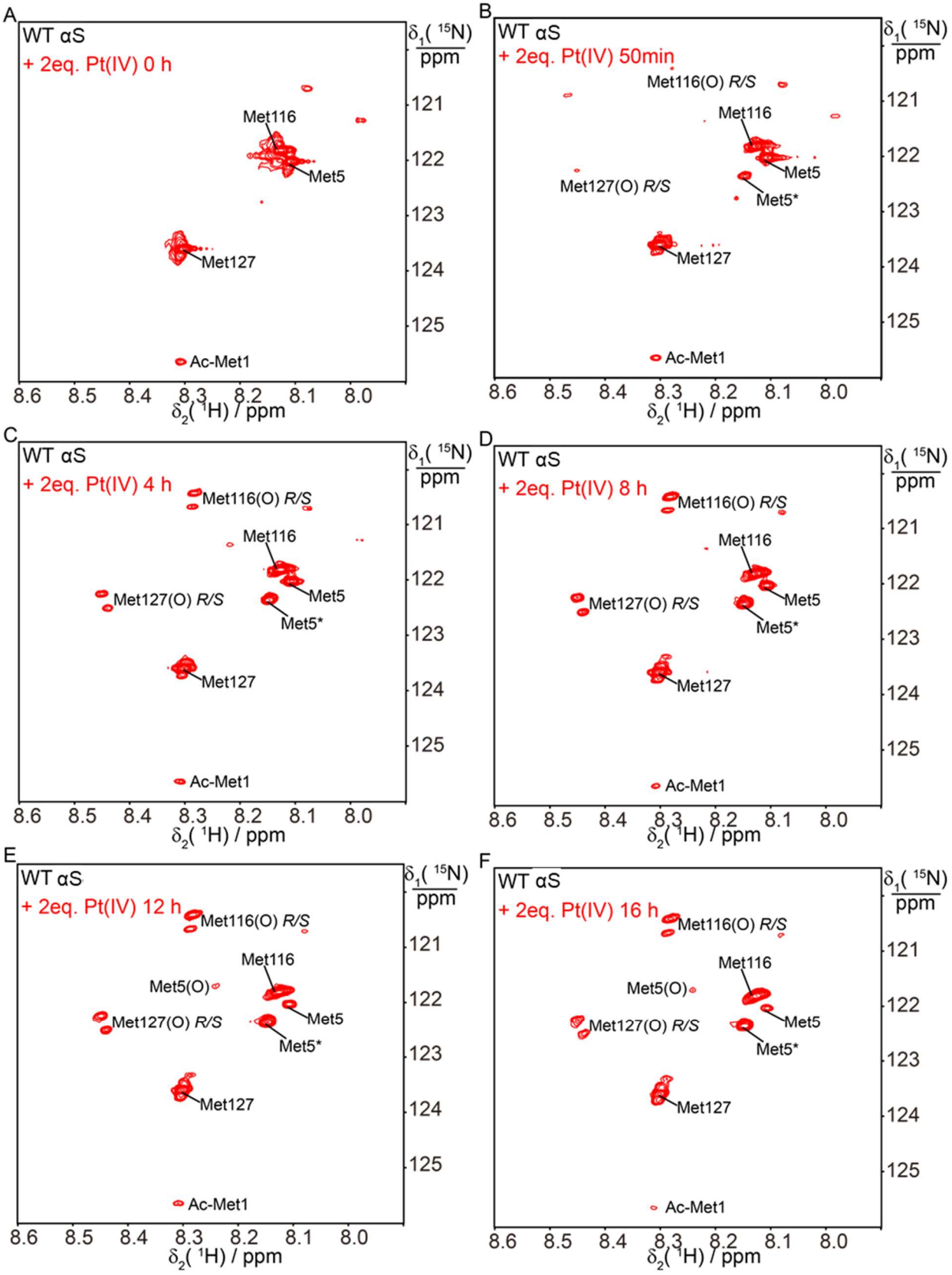


Figure S17. The products of 0.1 mM αS after incubation with 2.0 mM Pt(IV) for different time at 25°C were characterized by ESI-Q-TOF.


A
WT αS
+ 2eq. Pt(IV) 0 h
Met116
Met5
Met127
Ac-Met1
B
WT αS
+ 2eq. Pt(IV) 50min
Met116(O) R/S
Met116
Met5
Met5*
Met127(O) R/S
Met127
Ac-Met1
C
WT αS
+ 2eq. Pt(IV) 4 h
Met116(O) R/S
Met116
Met5
Met5*
Met127(O) R/S
Met127
Ac-Met1
D
WT αS
+ 2eq. Pt(IV) 8 h
Met116(O) R/S
Met116
Met5
Met5*
Met127(O) R/S
Met127
Ac-Met1
E
WT αS
+ 2eq. Pt(IV) 12 h
Met116(O) R/S
Met116
Met5(O)
Met5
Met5*
Met127(O) R/S
Met127
Ac-Met1
F
WT αS
+ 2eq. Pt(IV) 16 h
Met116(O) R/S
Met116
Met5(O)
Met5
Met5*
Met127(O) R/S
Met127
Ac-Met1
δ1(15N) ppm
121
122
123
124
125
8.6 8.5 8.4 8.3 8.2 8.1 8.0
δ2(1H) / ppm

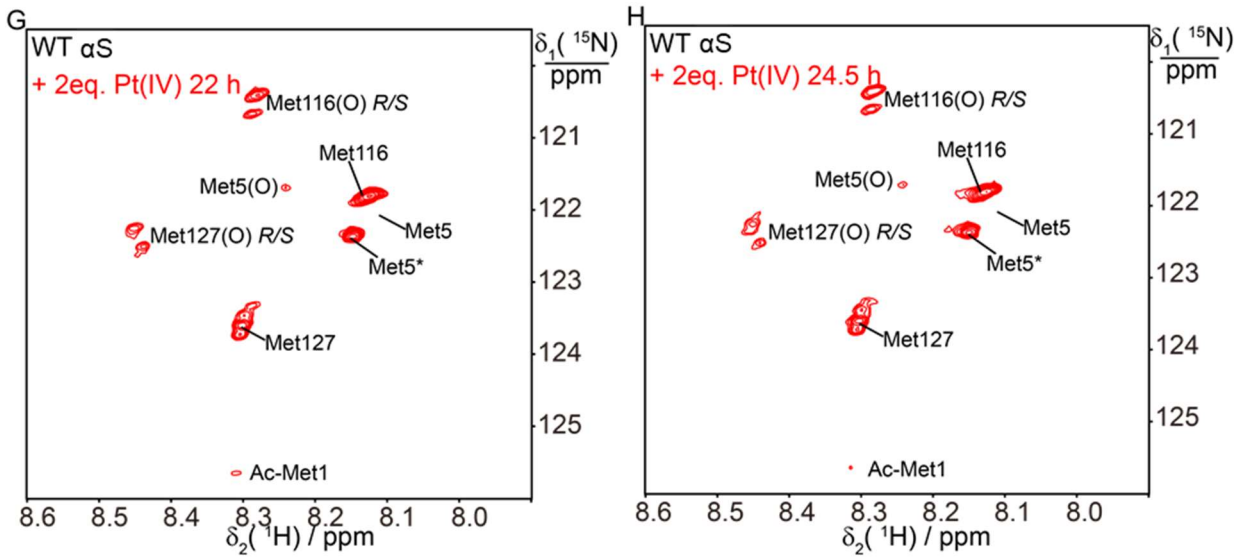


Figure S18. ^{1}H-^{15}N HSQC spectra recorded for 0.15 mM ^{15}N-Met enriched αS after incubation with 0.3 mM Pt(IV) from 0 h to 24.5 h in 20 mM MES, pH 6.4 and 298 K.

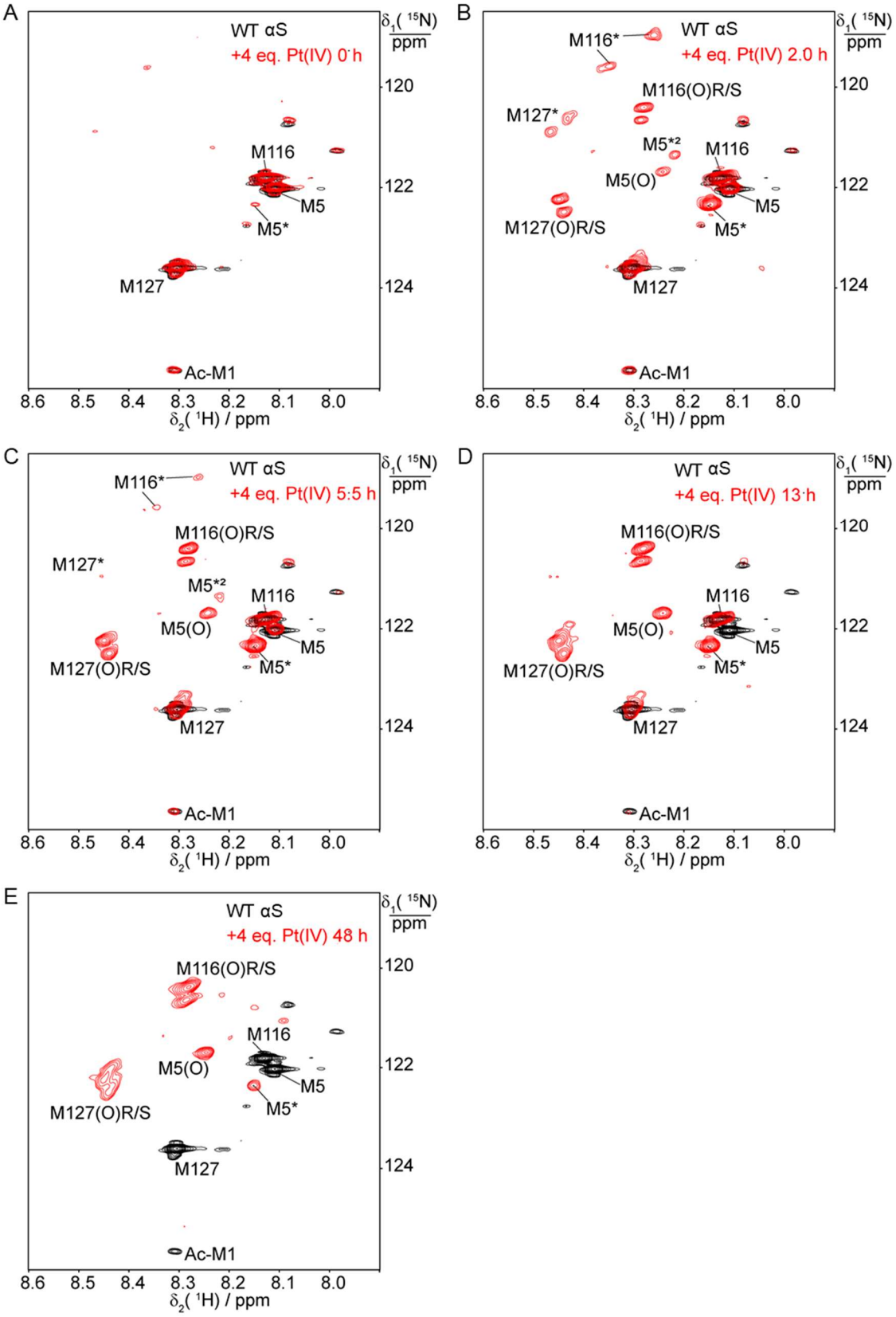
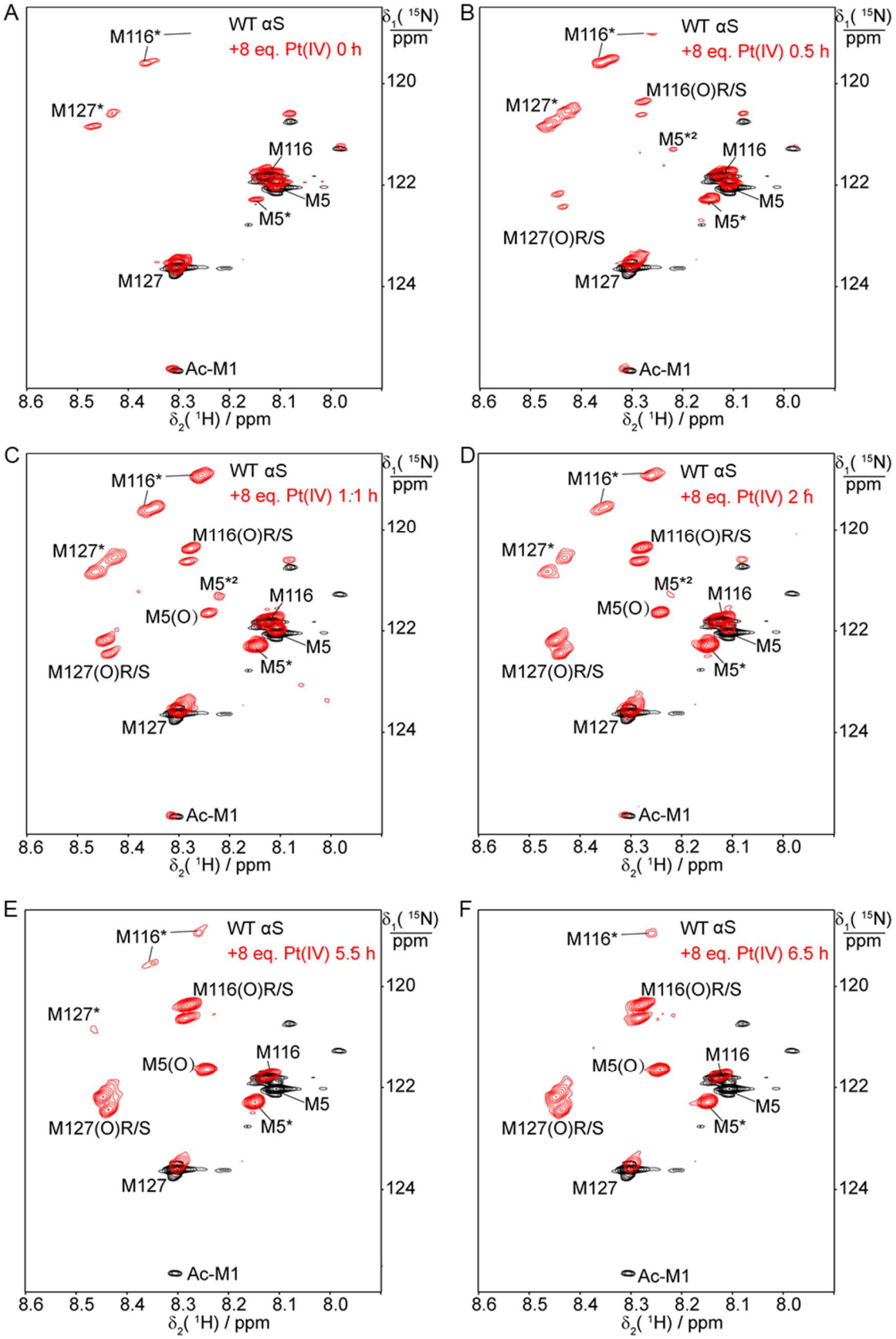


Figure S19. Overlay of ^{1}H-^{15}N HSQC spectra recorded for 0.15 mM ^{15}N-methionine labeled αS (black) and 0.15 mM ^{15}N-methionine enriched αS incubated with 4 folds of Pt(IV) for different time at 298 K (red). The M5*and M5*^{2} indicate two resonances formed by the M5 because of oxidation of M116 or M127 at the C-terminus.


A
WT αS
+8 eq. Pt(IV) 0 h
M116*
M127*
M116
M5
M5*
M127
Ac-M1
B
WT αS
+8 eq. Pt(IV) 0.5 h
M116*
M116(O)R/S
M127*
M5*²
M116
M5
M5*
M127(O)R/S
M127
Ac-M1
C
WT αS
+8 eq. Pt(IV) 1.1 h
M116*
M116(O)R/S
M127*
M5*²
M116
M5(O)
M5
M5*
M127(O)R/S
M127
Ac-M1
D
WT αS
+8 eq. Pt(IV) 2 h
M116*
M116(O)R/S
M127*
M5*²
M116
M5(O)
M5
M5*
M127(O)R/S
M127
Ac-M1
E
WT αS
+8 eq. Pt(IV) 5.5 h
M116*
M116(O)R/S
M127*
M116
M5(O)
M5
M5*
M127(O)R/S
M127
Ac-M1
F
WT αS
+8 eq. Pt(IV) 6.5 h
M116*
M116(O)R/S
M116
M5(O)
M5
M5*
M127(O)R/S
M127
Ac-M1
δ1(15N) ppm
120
122
124
8.6 8.5 8.4 8.3 8.2 8.1 8.0
δ2(1H) / ppm

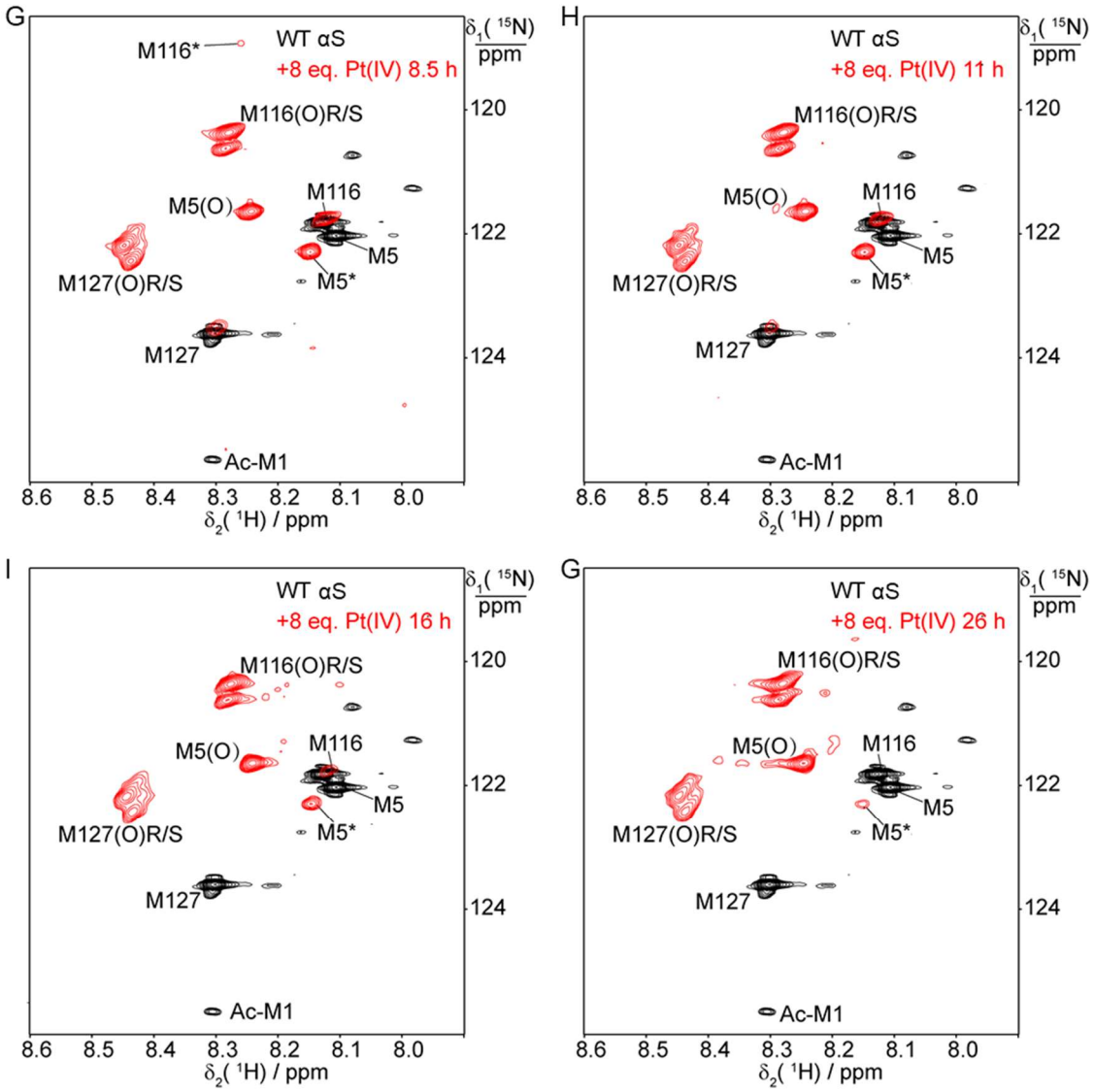


Figure S20. Overlay of ^{1}H-^{15}N HSQC spectra recorded for 0.15 mM ^{15}N-methionine labeled αS (black) and 0.15 mM ^{15}N-methionine enriched αS incubated with 8 folds of Pt(IV) for different time at 298 K (red). The cross-peaks of M116* were not displayed due to narrow spectrum width in the first two spectra. The M5*and M5*^{2} indicate two new resonances formed by the M5 because of oxidation of C-terminal M116 or M127. The Ac-M1 denotes the N-acetylated M1.

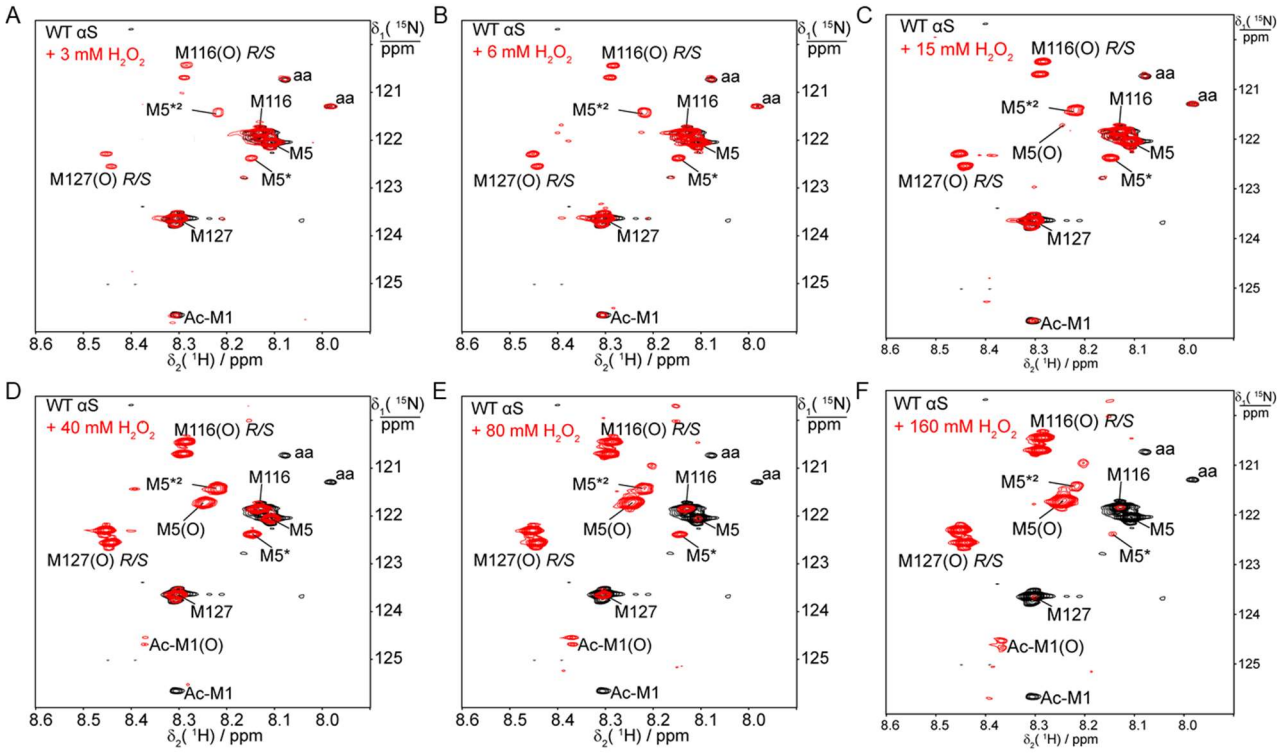


Figure S21. Overlay of the ^{1}H-^{15}N HSQC spectra recorded for the sample of 0.3 mM ^{15}N-Met enriched αS after incubation with different concentrations of H_2O_2 from 3 mM to 160 mM in 20 mM MES at pH 6.4 and 298K. The M5* and M5*^{2} indicate two resonances formed by the M5 because of oxidation of C-terminal M116 or M127. The Ac-M1 denotes the N-acetylated M1, and the aa represents cross-peaks produced by amino scrambling from ^{15}N Met in the protein biosynthesis.

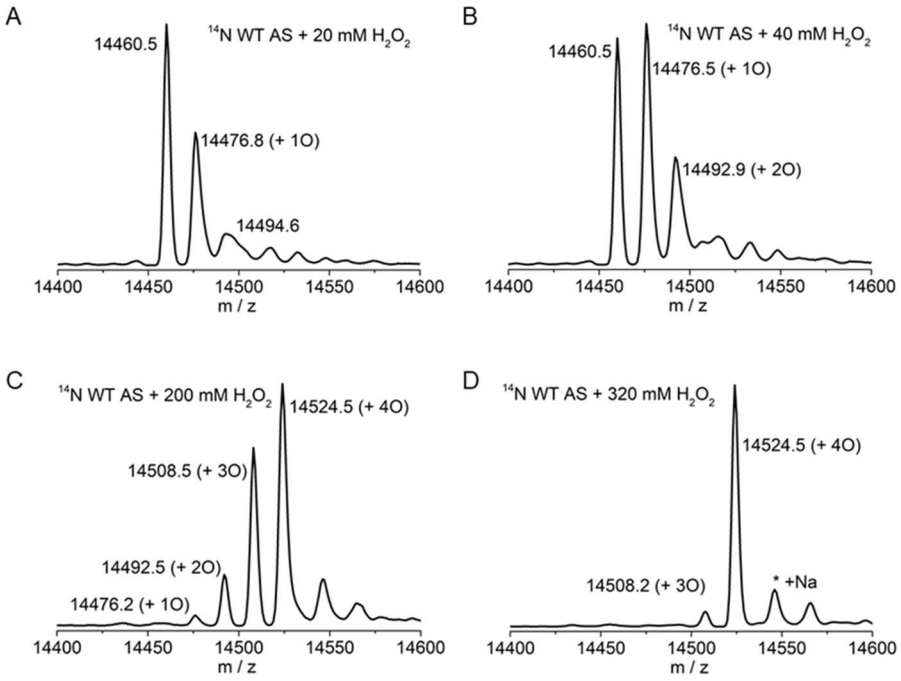


Figure S22. Mass spectra recorded for the mixture of αS after incubation with different concentrations of H_2O_2 at 25°C.

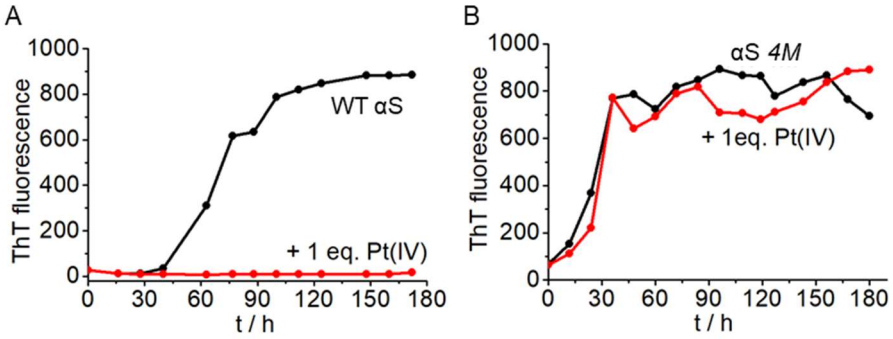


Figure S23. Fluorescence changes of ThT at 487 nm for the mixture of 0.1 mM αS and one equivalent of Pt(IV) during incubation at 37°C. (A) αS, (B) αS M1G/M5I/M116I/M127I (*4M*).

Table S1 Species with molecular mass determined in the mixture of 0.1 mM αS or its mutant after incubation with 0.1 mM Pt(IV) determined by the mass spectrometry.

	αS		αS M1G/M5I		αS M116I/M127I		αS M1G/M5IM116I/M127I	
	Theoretiacal mass (Dalton)	Observed mass	Theoretiacal mass	Observed mass	Theoretiacal mass	Observed mass	Theoretiacal mass	Observed mass
αS	14460.2	14460.2	14386.4	14386.4	14424.1	14424.2	14331.9	14332.4
αS+O	14476.2	14476.7	14402.4	14402.5				
αS+Pt	14653.2	14653.3	14579.4	14579.4				
αS+Pt+O	14669.2	14669.5	14595.4	14596.2				

Table S2 Species with molecular mass determined in the mixture of 0.1 mM αS or its mutant after incubation with 0.2 mM Pt(IV) determined by the mass spectrometry.

	αS		αS M1G/M5I		αS M116I/M127I	
	Theoretiacal mass (Dalton)	Observed mass	Theoretiacal mass	Observed mass	Theoretiacal mass	Observed mass
αS	14460.2	14460.5	14386.4	14386.4	14424.1	14424.2
αS+O	14476.2	14475.9	14402.4	14402.4	14440.1	14441.9
αS+2O	14492.2	14491.6	14418.4	14418.7		
αS+Pt	14653.2	14653.3	14579.4	14580.2	14617.1	14618.0
αS+Pt+O	14669.2	14669.4	14595.4	14595.1		
αS+Pt+2O	14685.2	14685.0				
αS+2Pt	14846.2	14846.4				
αS+2Pt-NH_3	14863.2	14863.4				
αS+2Pt-NH_3-O	14879.2	14878.3				

Table S3 Species with molecular mass determined in the mixture of 0.1 mM αS after incubation with 4, 8 and 20 equivalents of Pt(IV) determined by the mass spectrometry.

	αS + 4eq. Pt(IV)		αS + 8eq. Pt(IV)		αS + 20eq. Pt(IV)	
	Theoretiacal mass (Dalton)	Observed mass	Theoretiacal mass	Observed mass	Theoretiacal mass	Observed mass
αS	14460.2	14459.6	14460.2	14458.9	14460.2	14459.6
αS+O	14476.2	14476.1	14476.2	14474.5	14476.2	14475.1
αS+2O	14492.2	14490.6	14492.2	14490.5	14492.2	14490.4
αS+3O	14508.2	14506.5	14508.2	14507.0	14508.2	14506.6
αS+Pt	14653.2	14651.4	14653.2	14651.8	14653.2	-
αS+Pt+O	14669.2	14667.5	14669.2	14668.4	14669.2	14668.4
αS+Pt-NH_3+O	14686.3	14685.4	14686.3	14685.3	14686.3	14685.3
αS+Pt-NH_3+2O	14702.3	14701.7	14702.3	14702.1	14702.3	14701.9
αS+Pt-NH_3+3O	14718.3	14717.7	14718.3	14718.4	14718.3	14718.3
αS+2Pt	14846.2	14847.6	14846.2	-	14846.2	-
αS+2Pt-NH_3	14863.2	14863.7	14863.2	-	14863.2	-
αS+2Pt-NH_3-O	14879.2	14879.8	14879.2	-	14879.2	-
αS+2Pt-NH_3-2O	14895.2	14896.3	14895.2	-	14895.2	-

'-' Indicates that the species has not been determined due to low signal strength.