Supplementary materials for

Activity of nicotinic acid substituted nicotinic acid adenine dinucleotide phosphate (NAADP) analogs in a human cell line: difference in specificity between human and sea urchin NAADP receptors.

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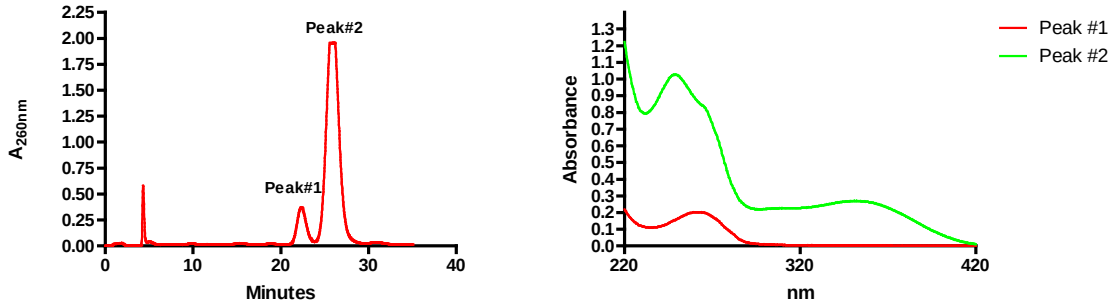
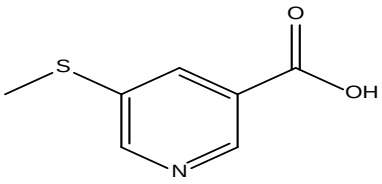
Contents:

Figure S1. HPLC purification of caged NAADP and UV spectrum of each peak

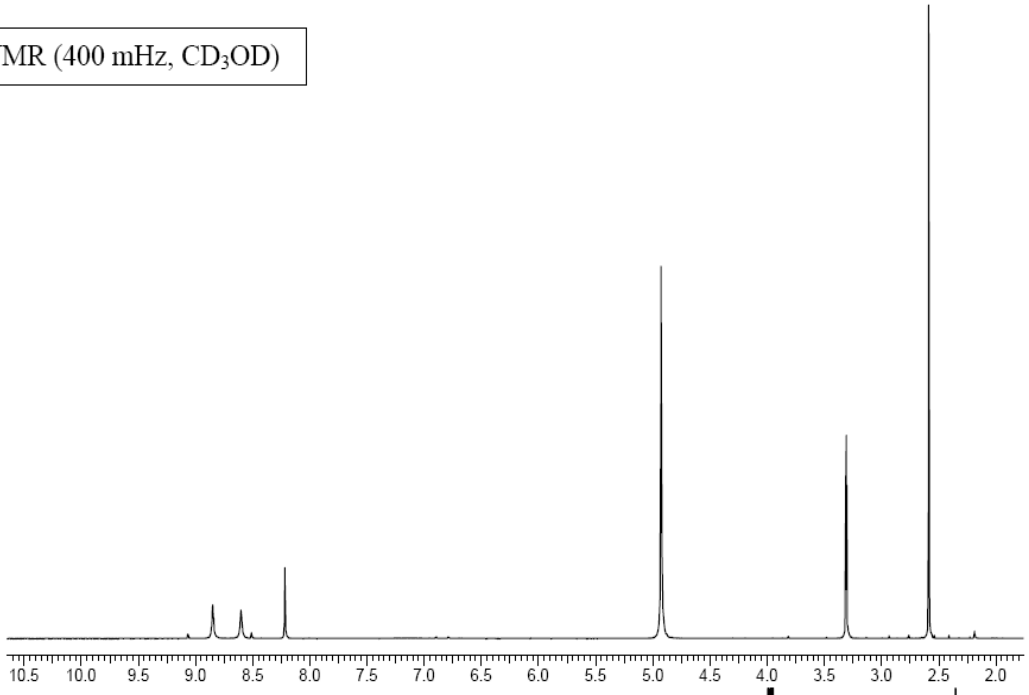


Separation of caged NAADP from contaminating NAADP. Left Panel: Caged NAADP was separated from NAADP by chromatography on an AG MP-1 column (BioRad Laboratories, Hercules, CA) using a gradient formed between water and 100 mM aqueous TFA [*Anal. Biochem*. 116 (1981) 357]. NAADP (Peak #1) eluted before caged NAADP (Peak #2). Right Panel: The identities of the peaks were confirmed by determining their UV spectra. Only Peak #2 showed the long wavelength absorption associated with the caging group. Peak #1 showed the typical UV absorption spectrum of NAADP.

Figure S2. Structure, ^{1}H NMR, ^{13}C NMR, and HRMS of 5-Thiomethylnicotinic acid



^{1}H NMR (400 mHz, CD_3OD)



^{13}C NMR (100 mHz, CD_3OD)

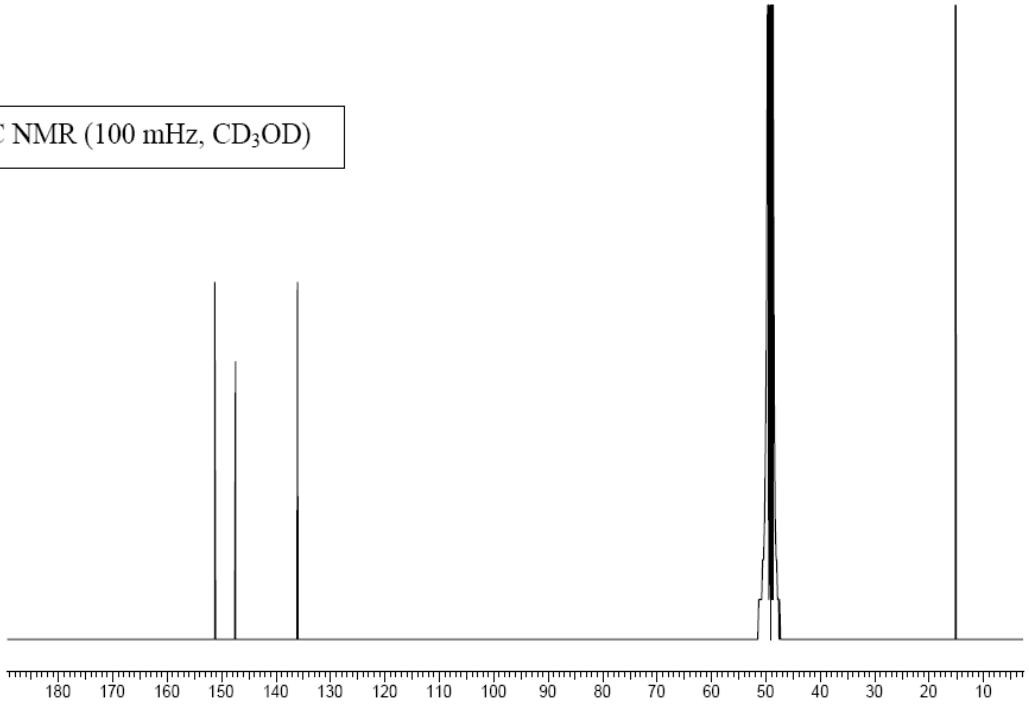


Figure S2 continued

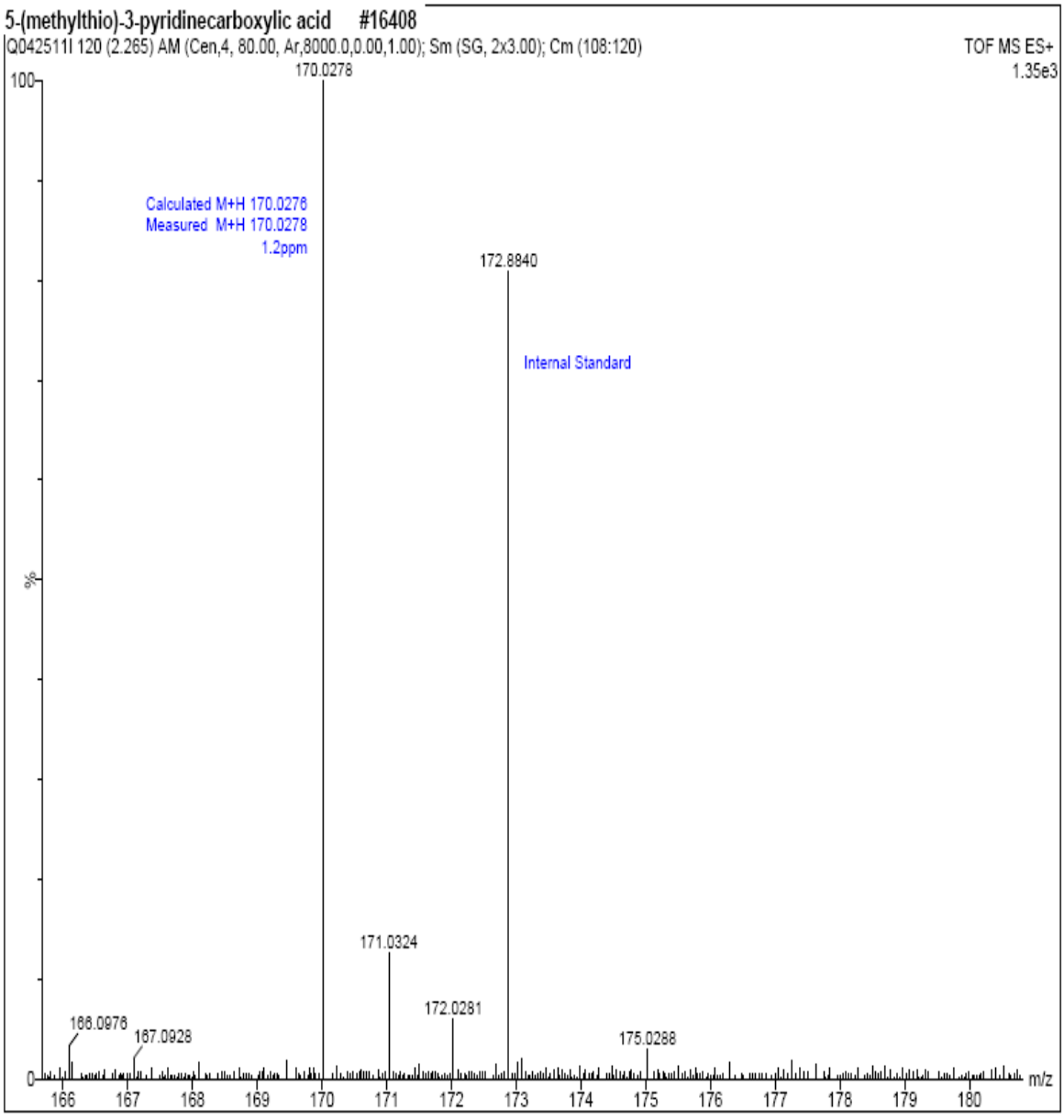
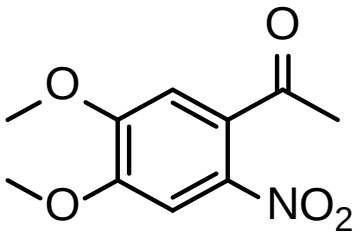


Figure S3. Structure and ^{1}H NMR of 4,5–dimethoxy-2-nitroacetophenone



^{1}H NMR (600 mHz, $CDCl_3$)

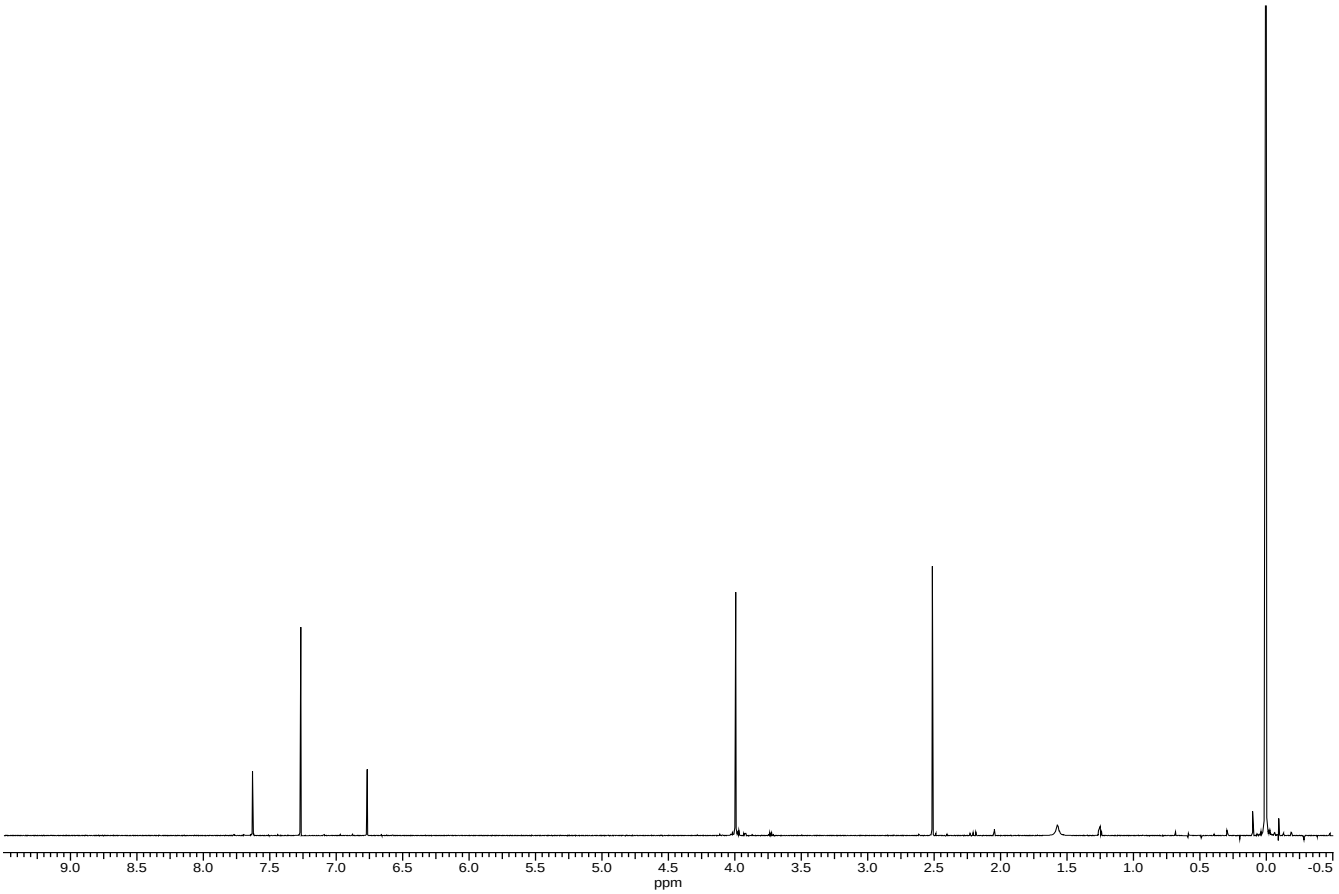
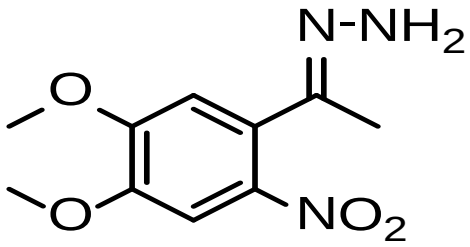


Figure S4. Structure and ^{1}H NMR of 4,5–dimethoxy-2- nitroacetophenylhydrazone



^{1}H NMR (600 mHz, $CDCl_3$)

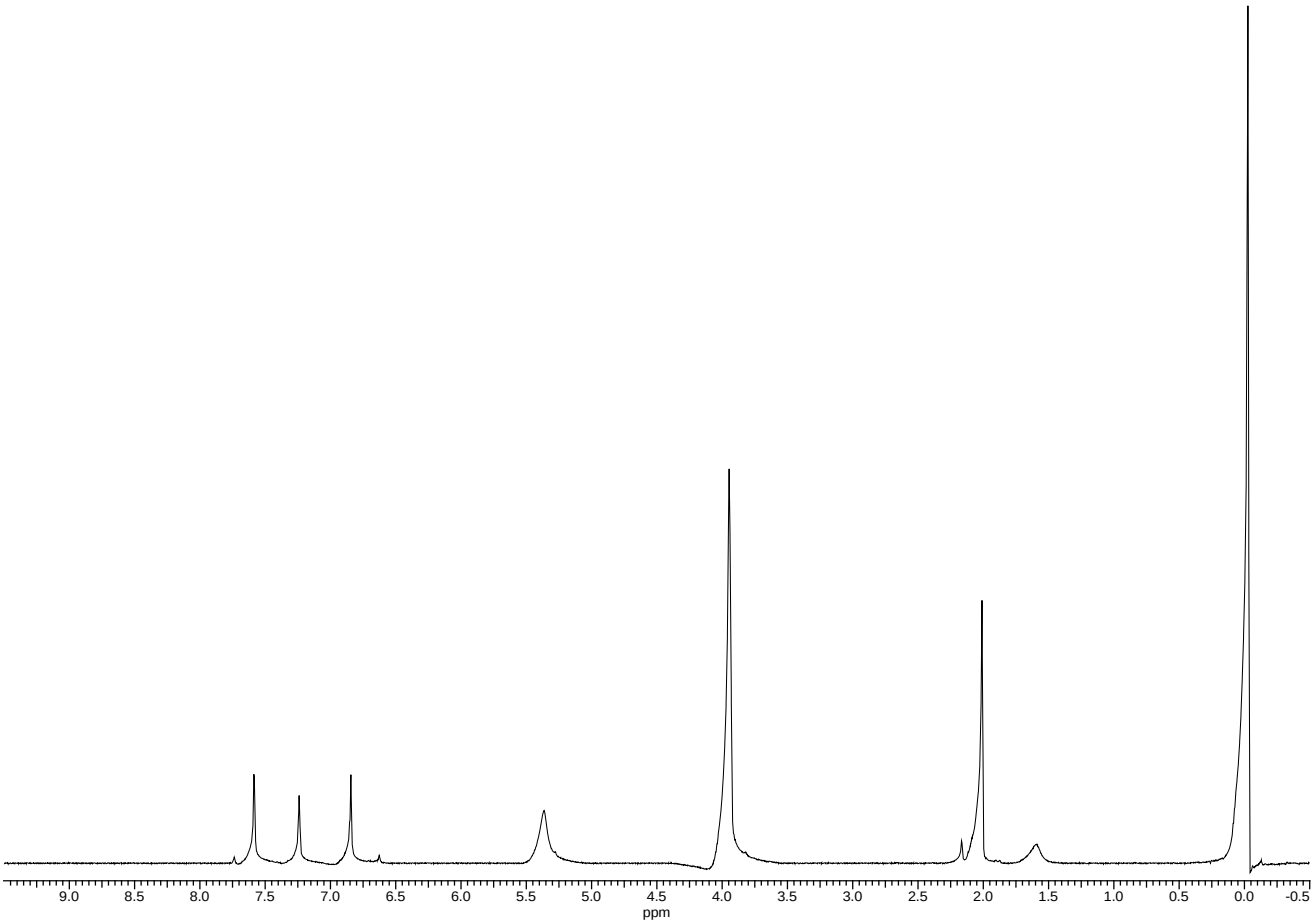
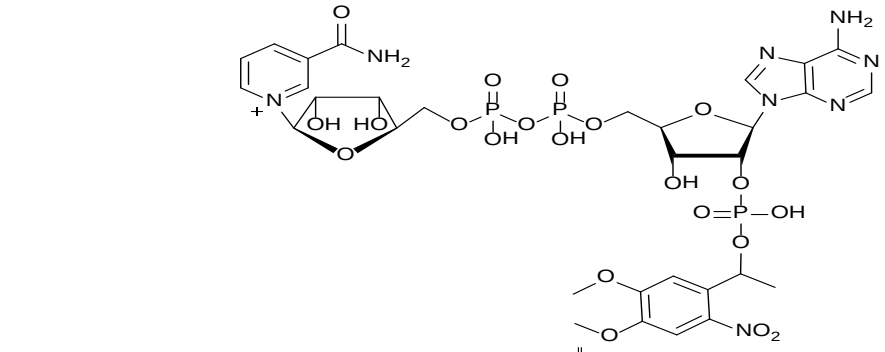
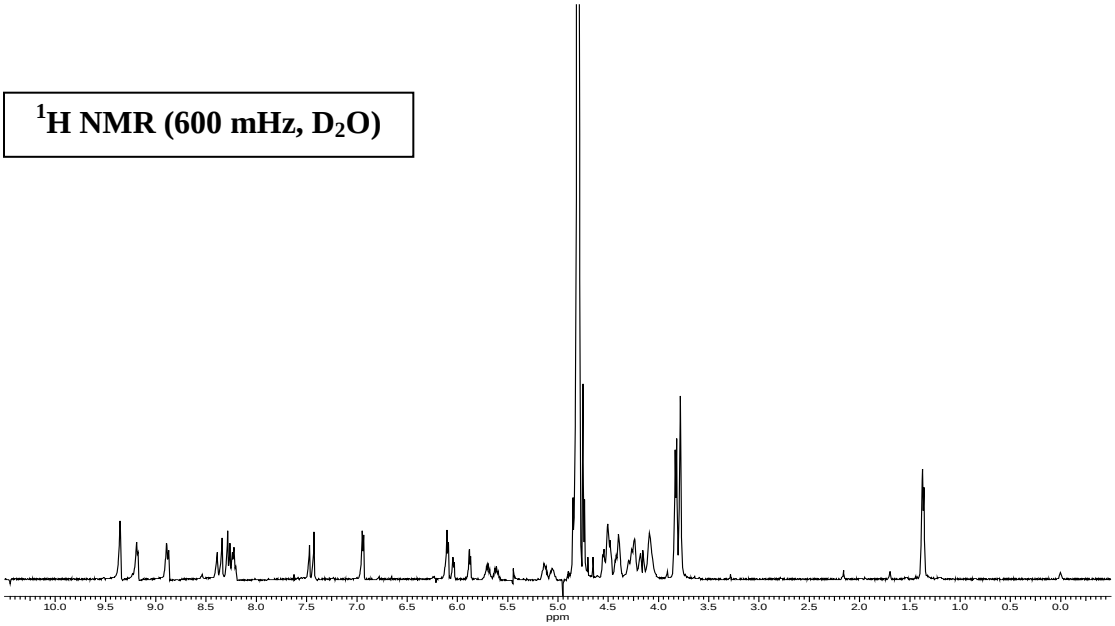


Figure S5. Structure, ^{1}H NMR, and ^{31}P NMR of DMNPE-caged NADP



^{1}H NMR (600 mHz, D_2O)



^{31}P NMR (162 mHz, D_2O)

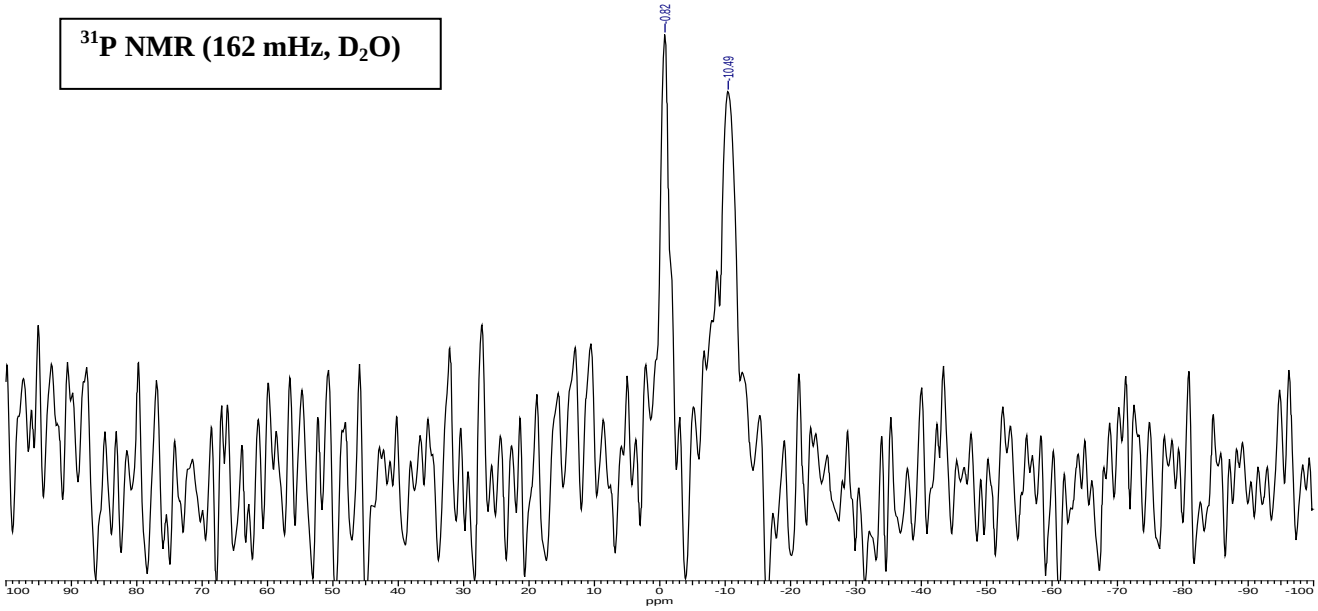
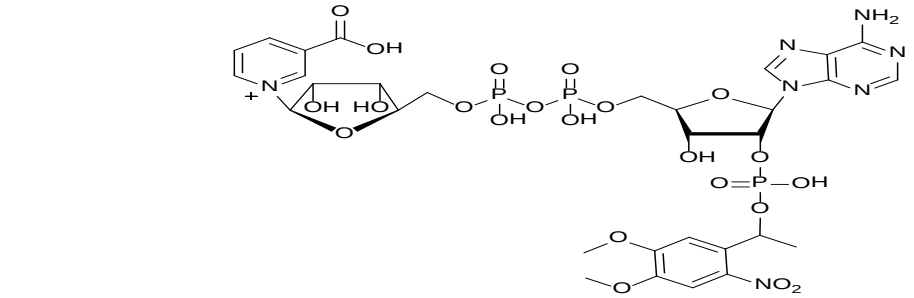
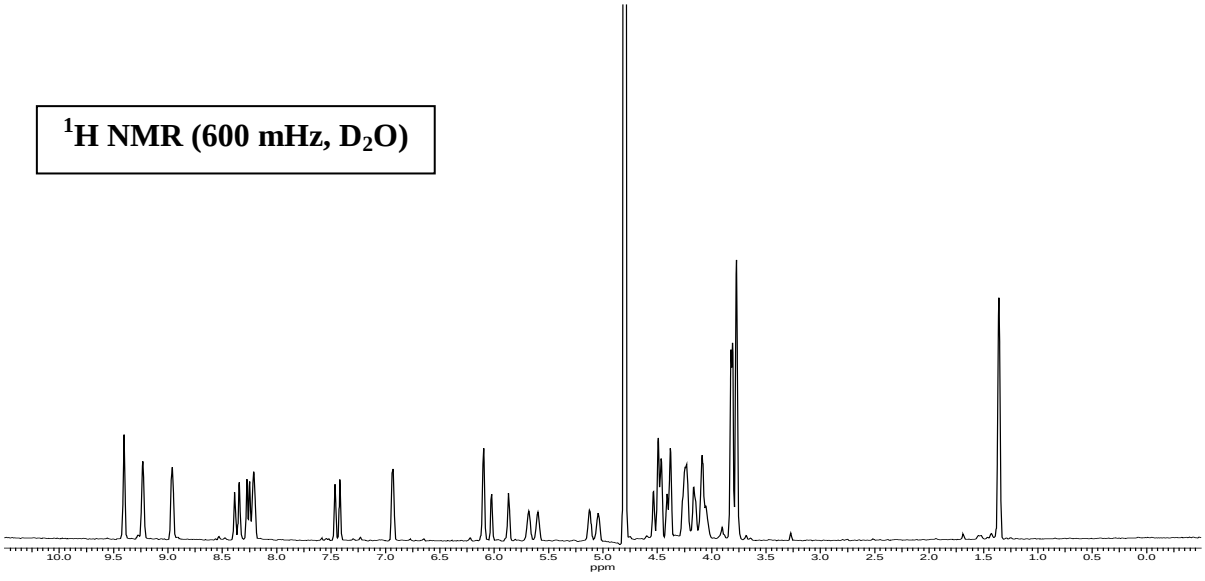


Figure S6. Structure, ^{1}H NMR, ^{31}P NMR, HPLC trace, and HRMS of caged NAADP



^{1}H NMR (600 mHz, D_2O)



^{31}P NMR (162 mHz, D_2O)

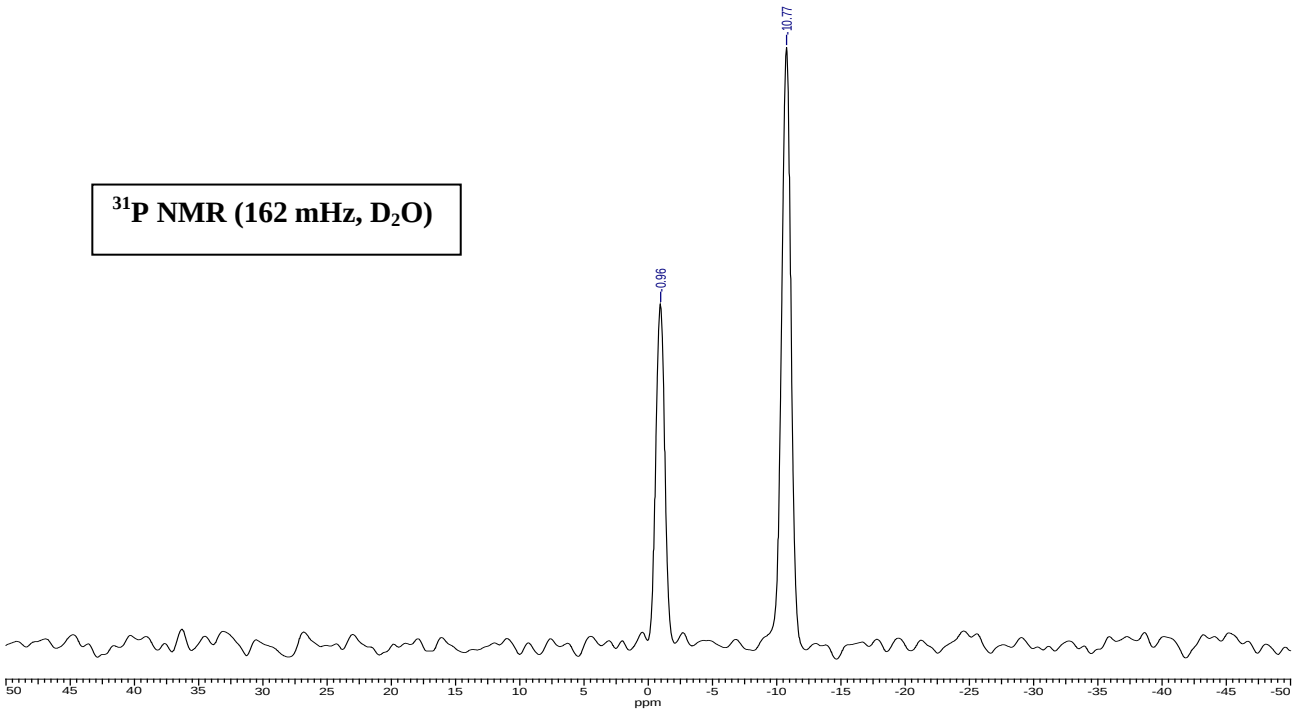
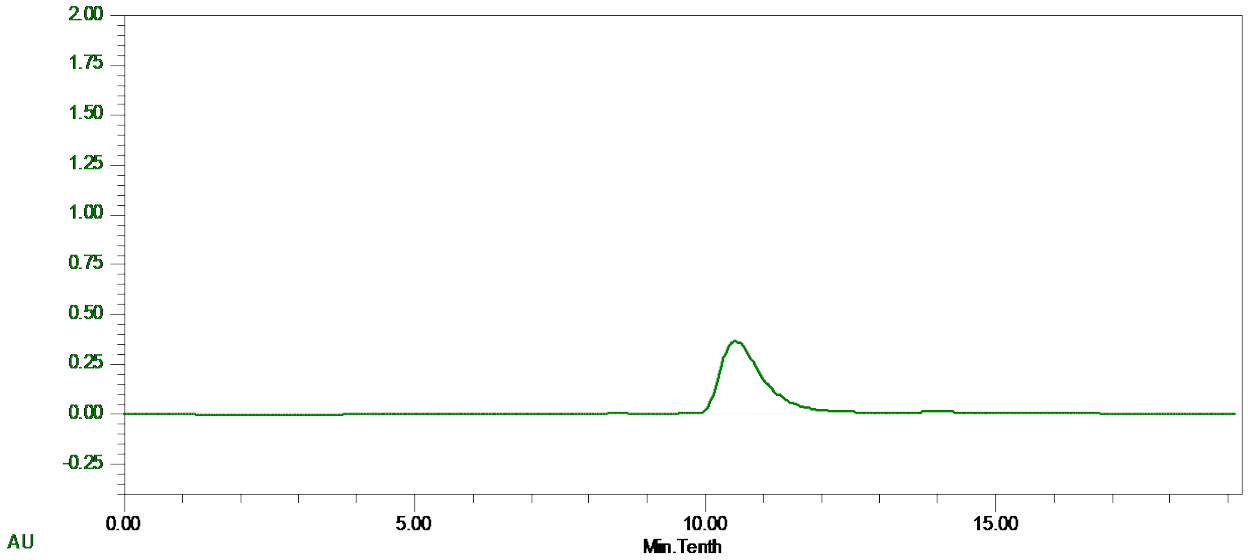


Figure S6 continued



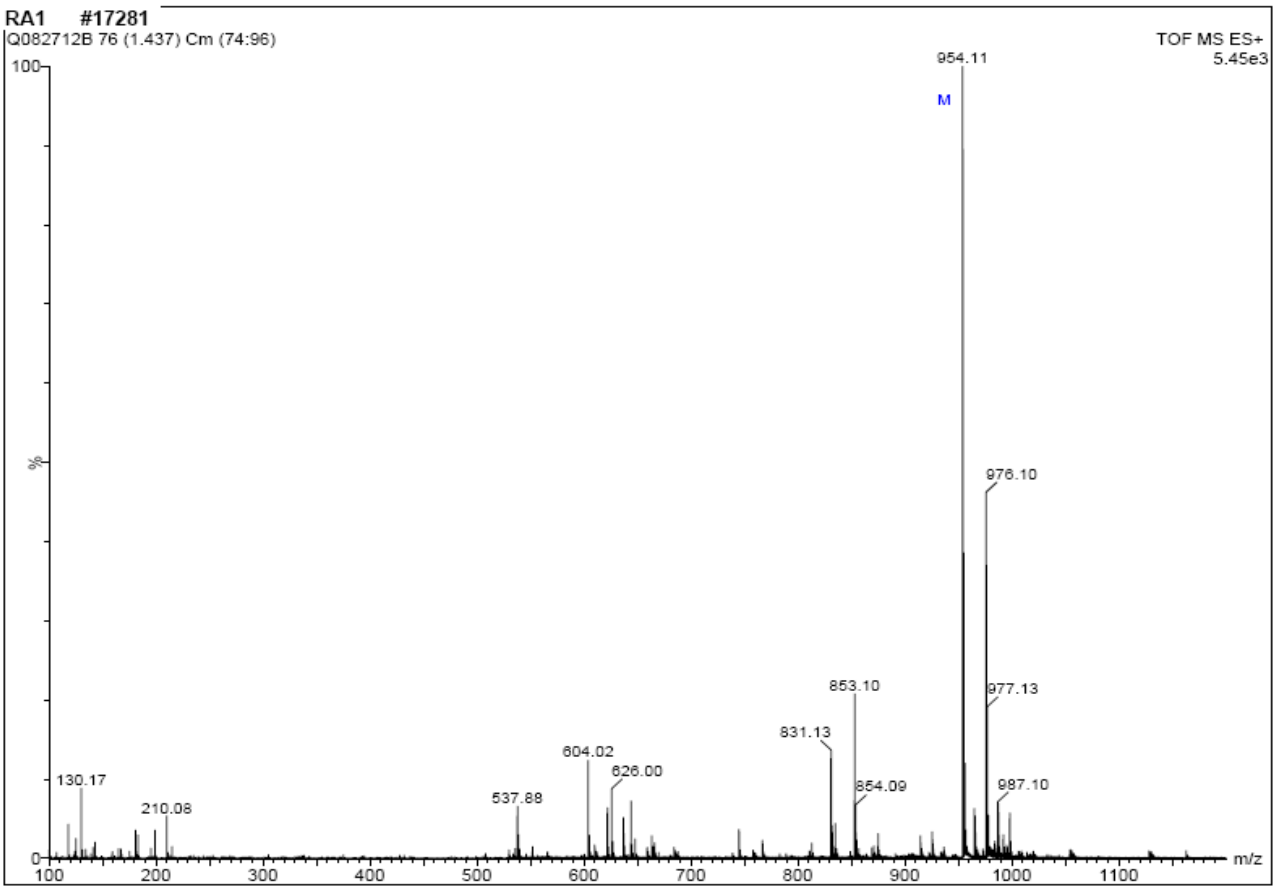
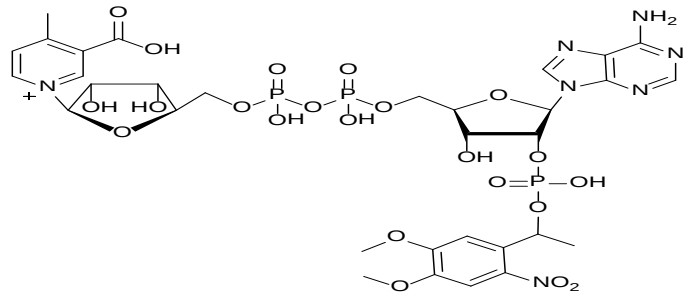
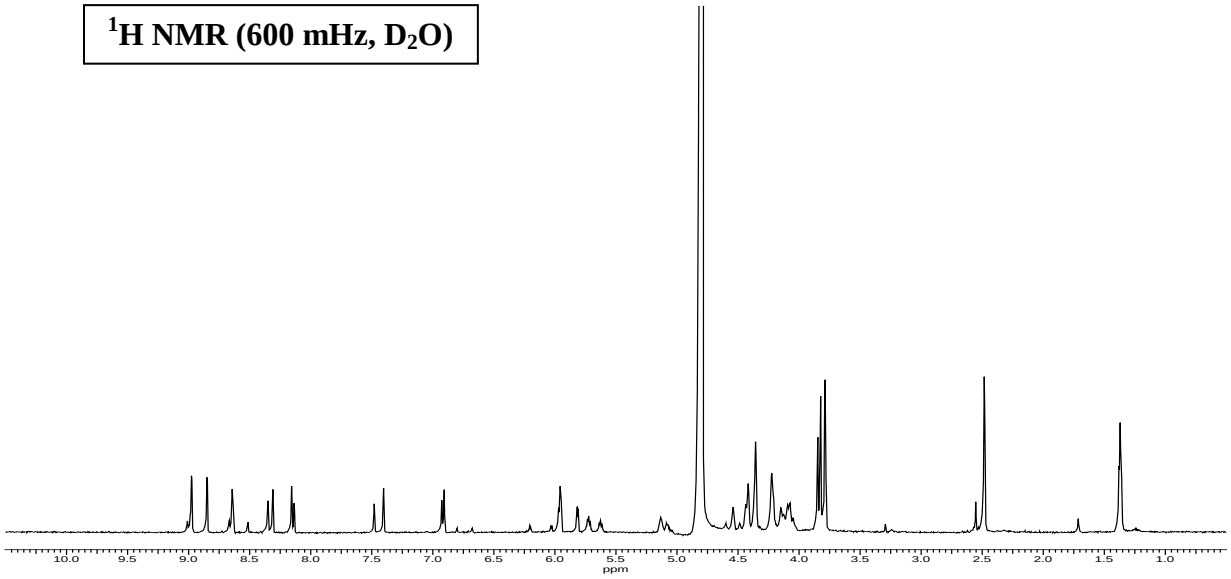


Figure S7. Structure, ^{1}H NMR, ^{31}P NMR, HPLC trace, and HRMS of caged 4-methyl-NAADP



^{1}H NMR (600 mHz, D_2O)



^{31}P NMR (162 mHz, D_2O)

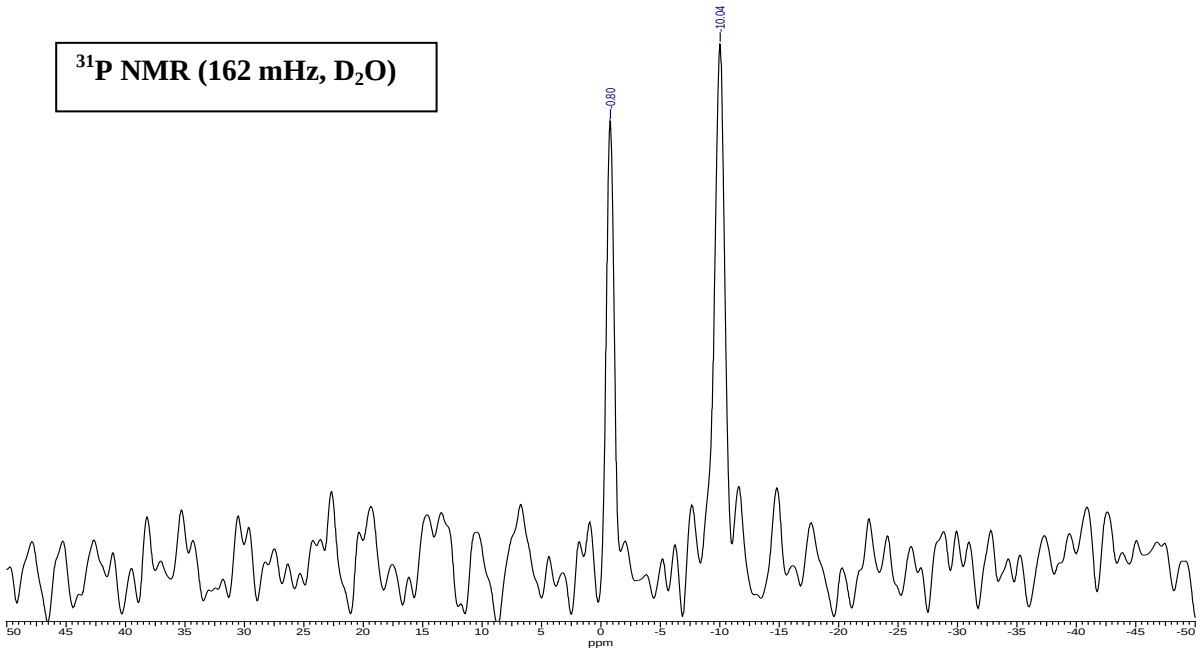
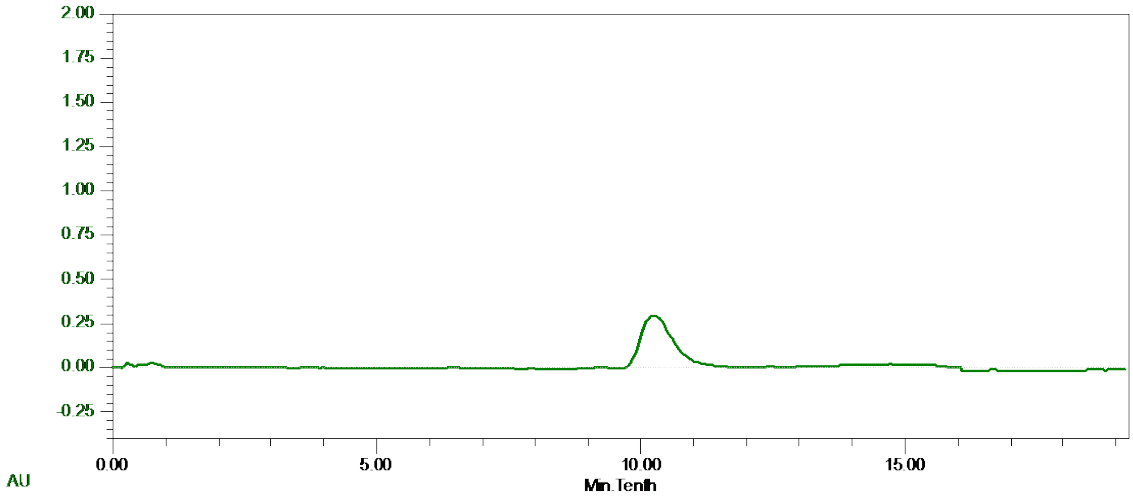


Figure S7 continued



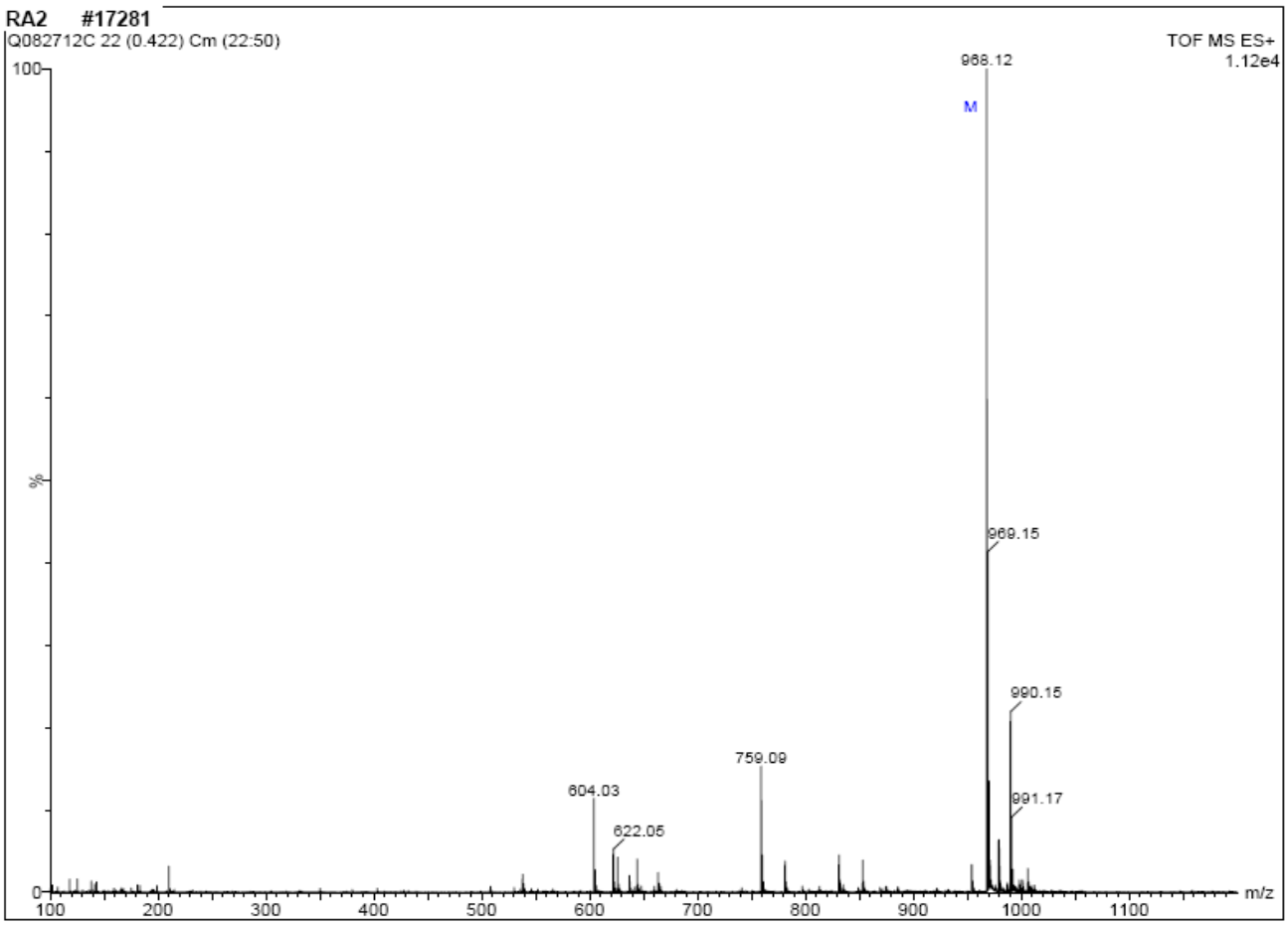
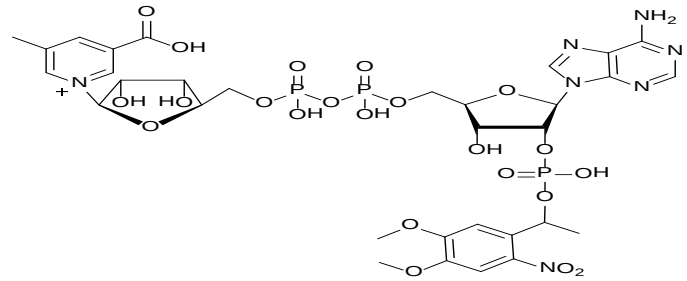
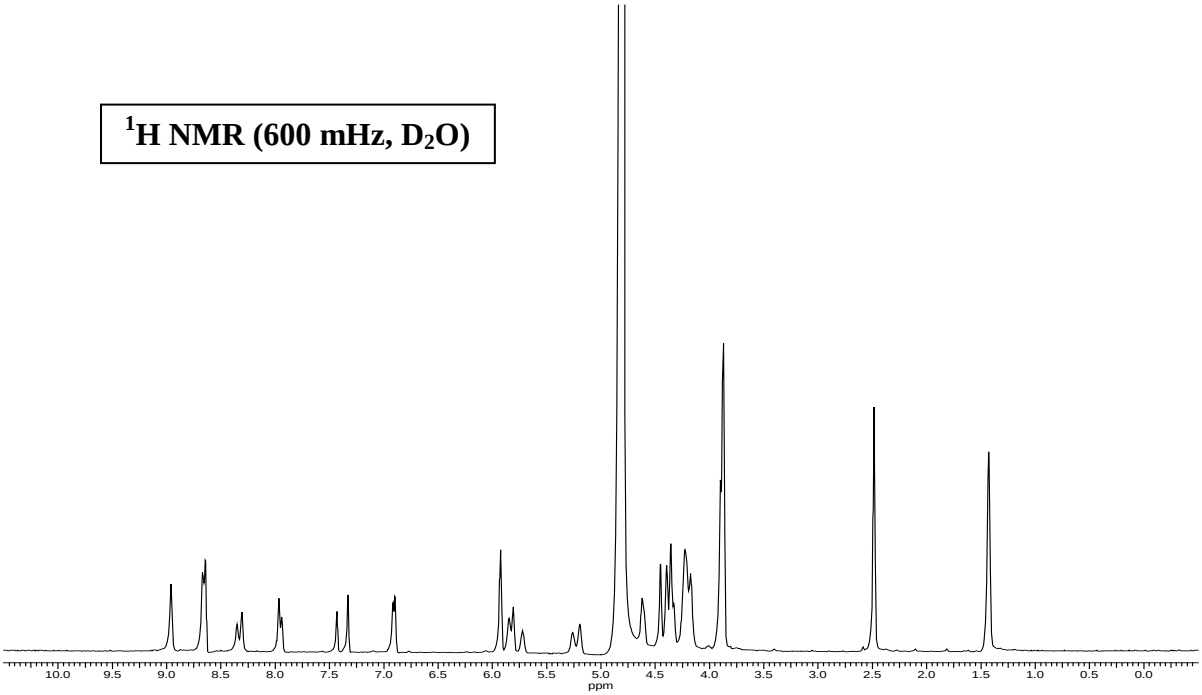


Figure S8. Structure, ^{1}H NMR, ^{31}P NMR, HPLC trace, and HRMS of caged 5-methyl-NAADP



^{1}H NMR (600 mHz, D_2O)



^{31}P NMR (162 mHz, D_2O)

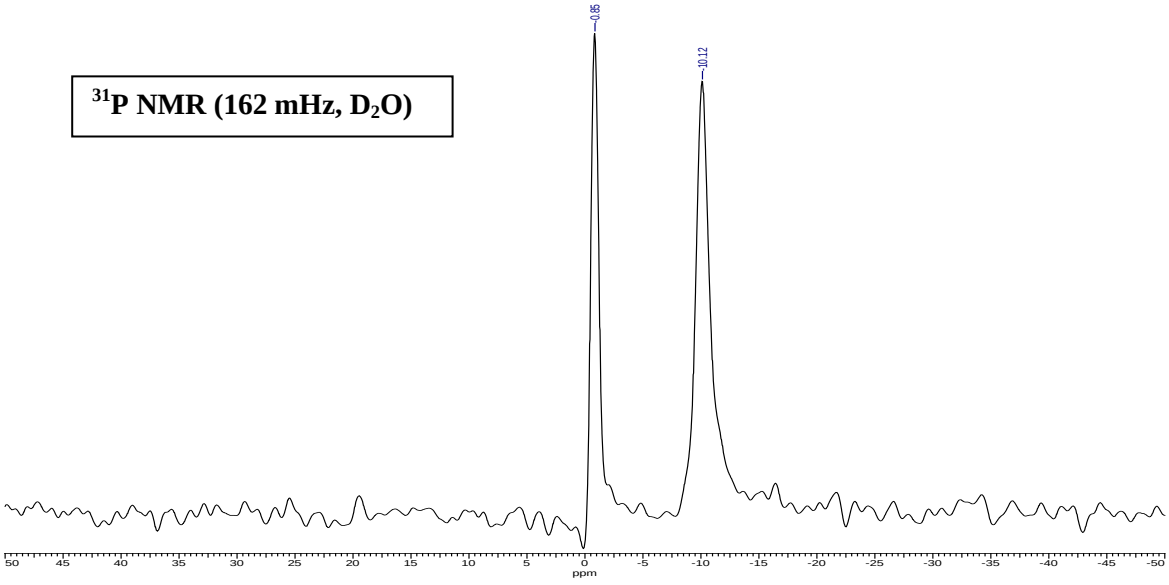
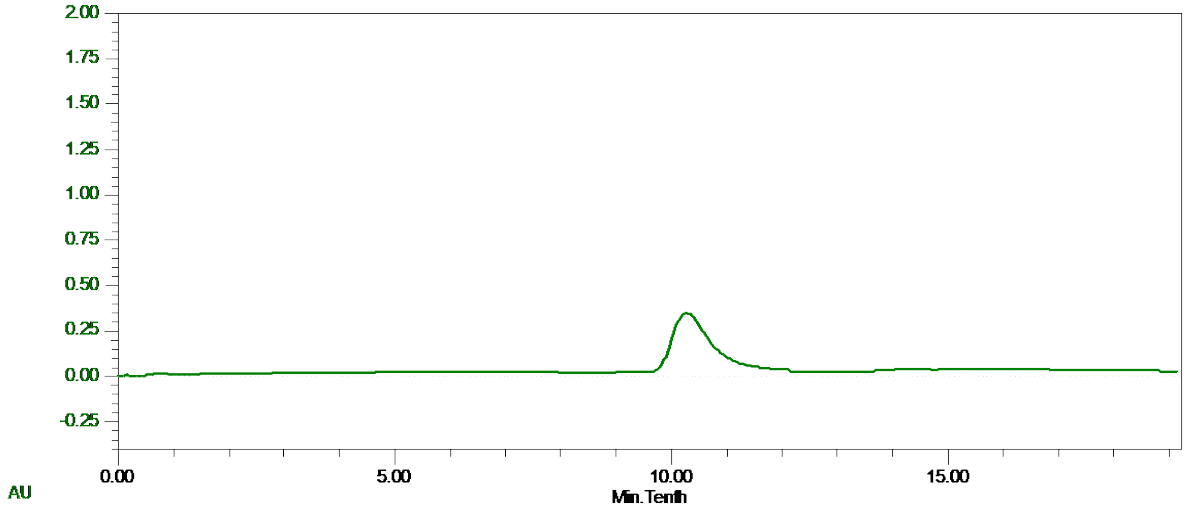


Figure S8 continued



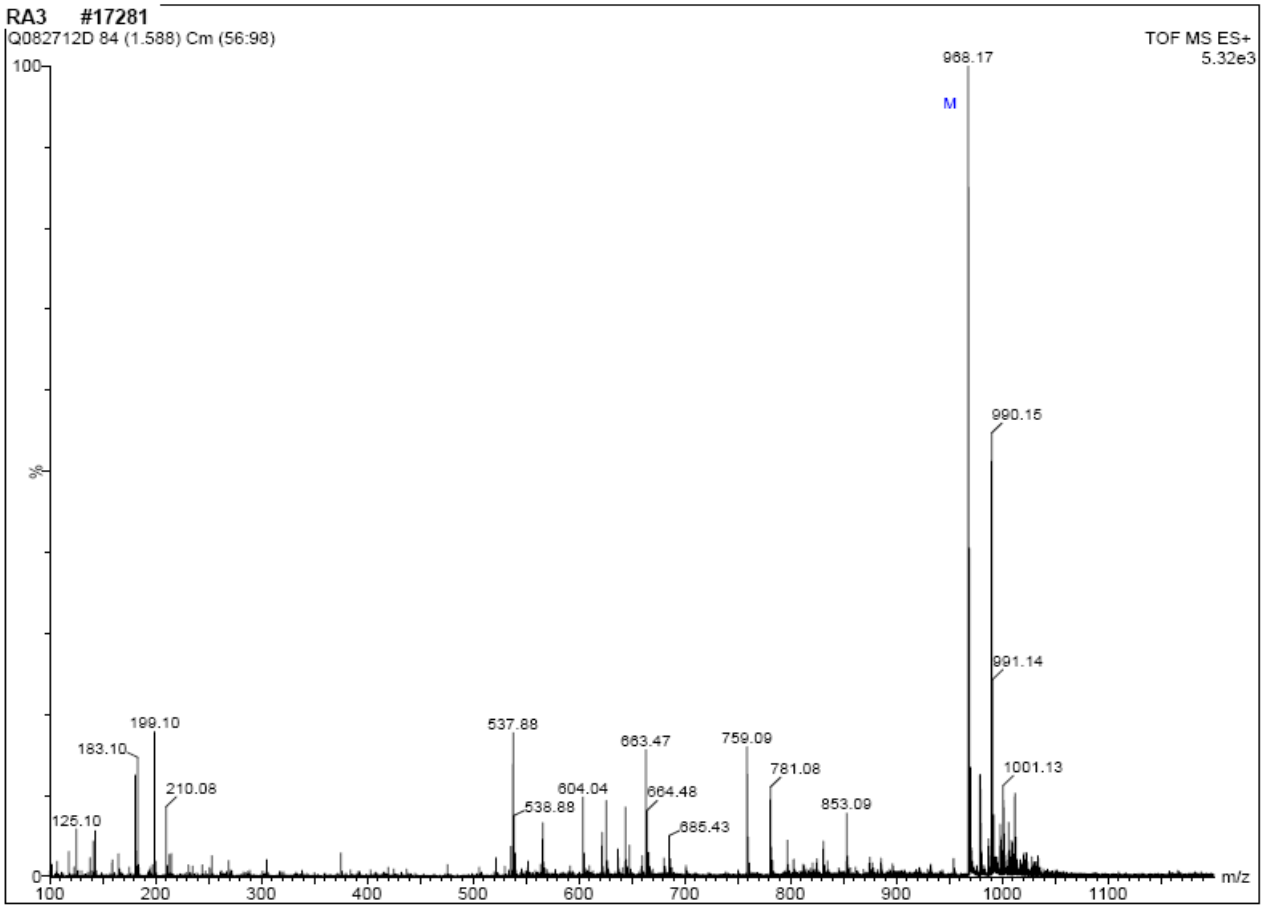
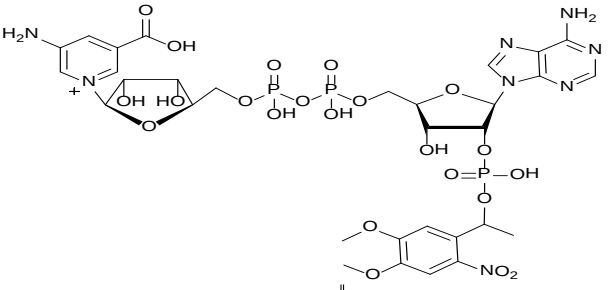
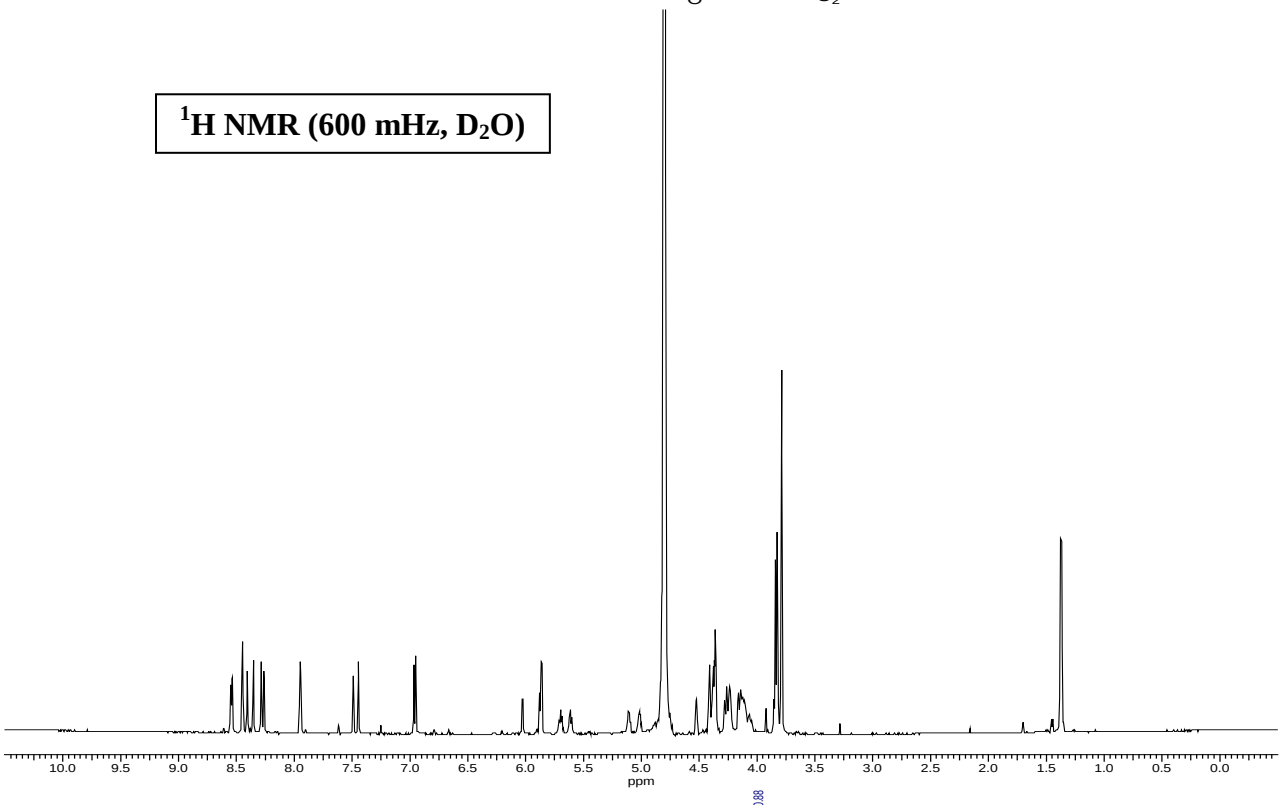


Figure S9. Structure, ^{1}H NMR, ^{31}P NMR, HPLC trace, and HRMS of caged 5-amino-NAADP



^{1}H NMR (600 mHz, D_2O)



^{31}P NMR (162 mHz, D_2O)

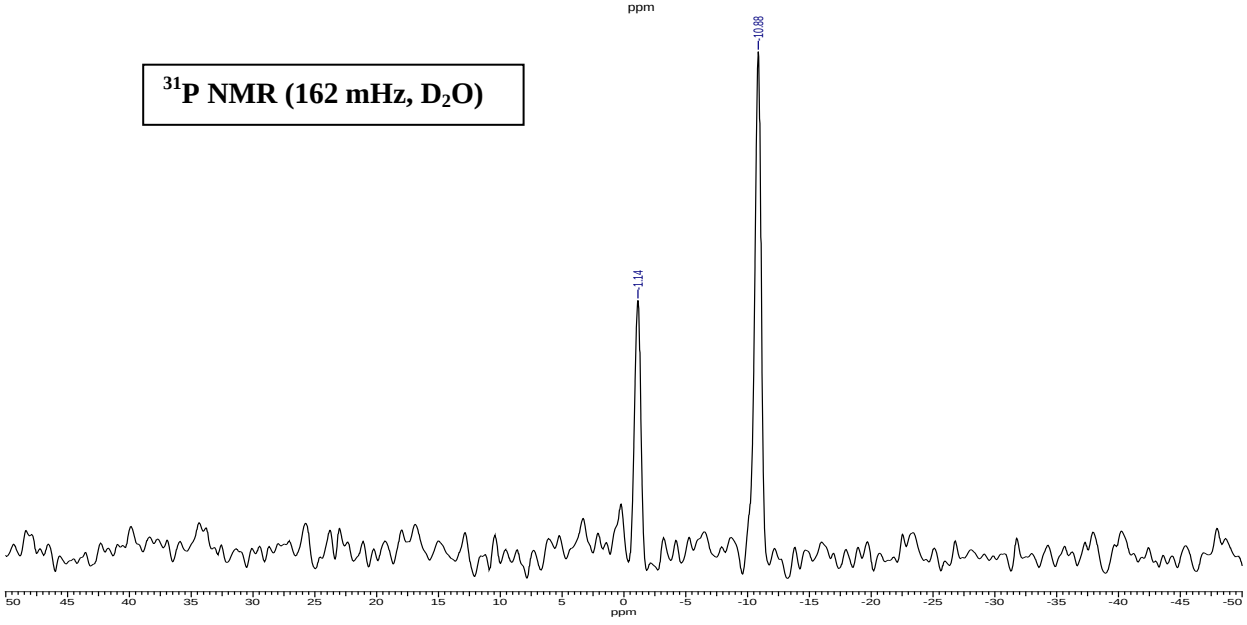
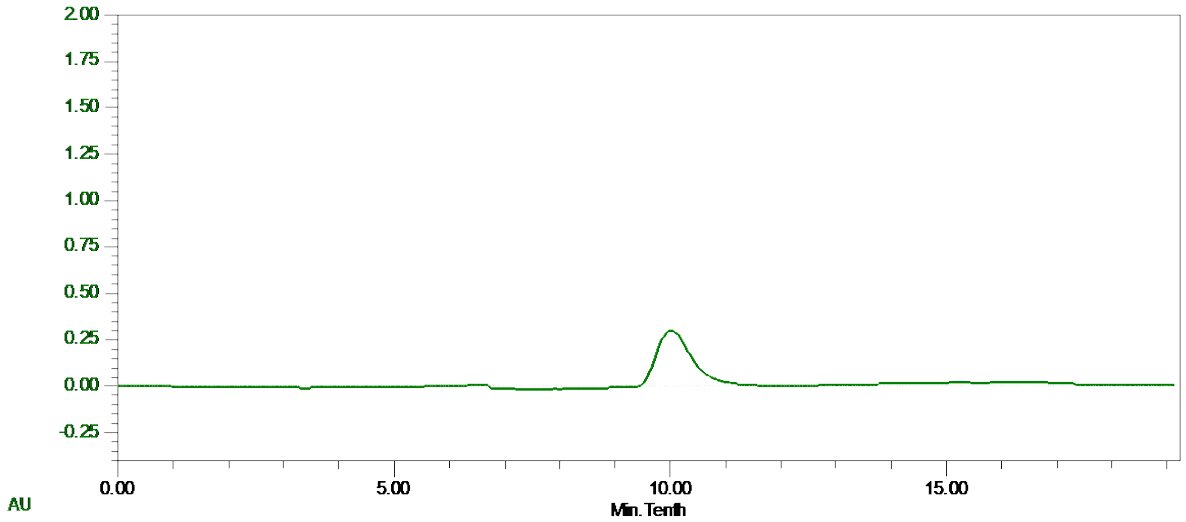


Figure S9 continued



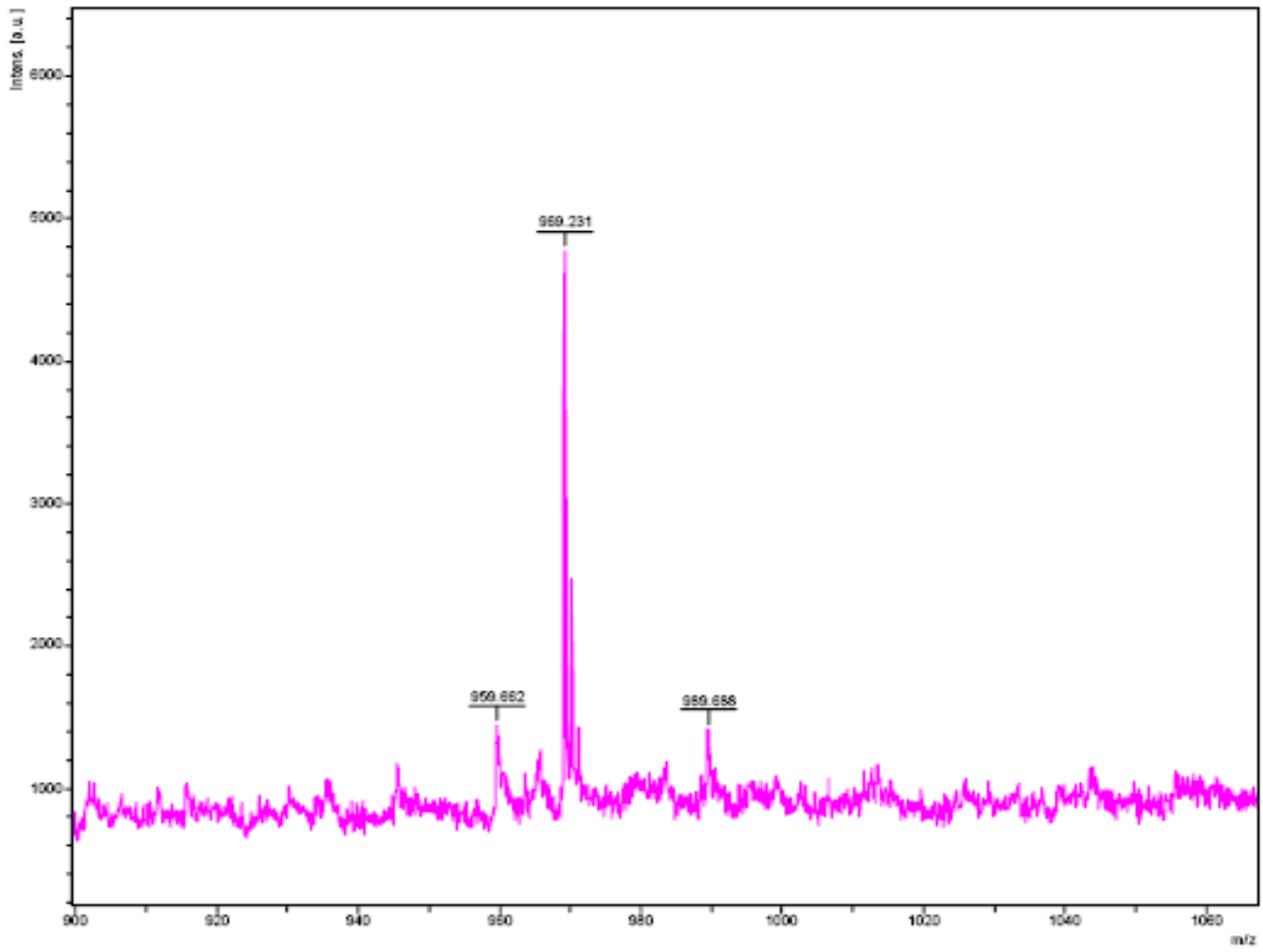
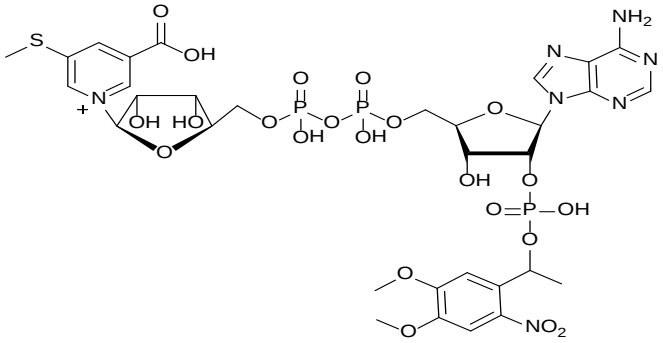
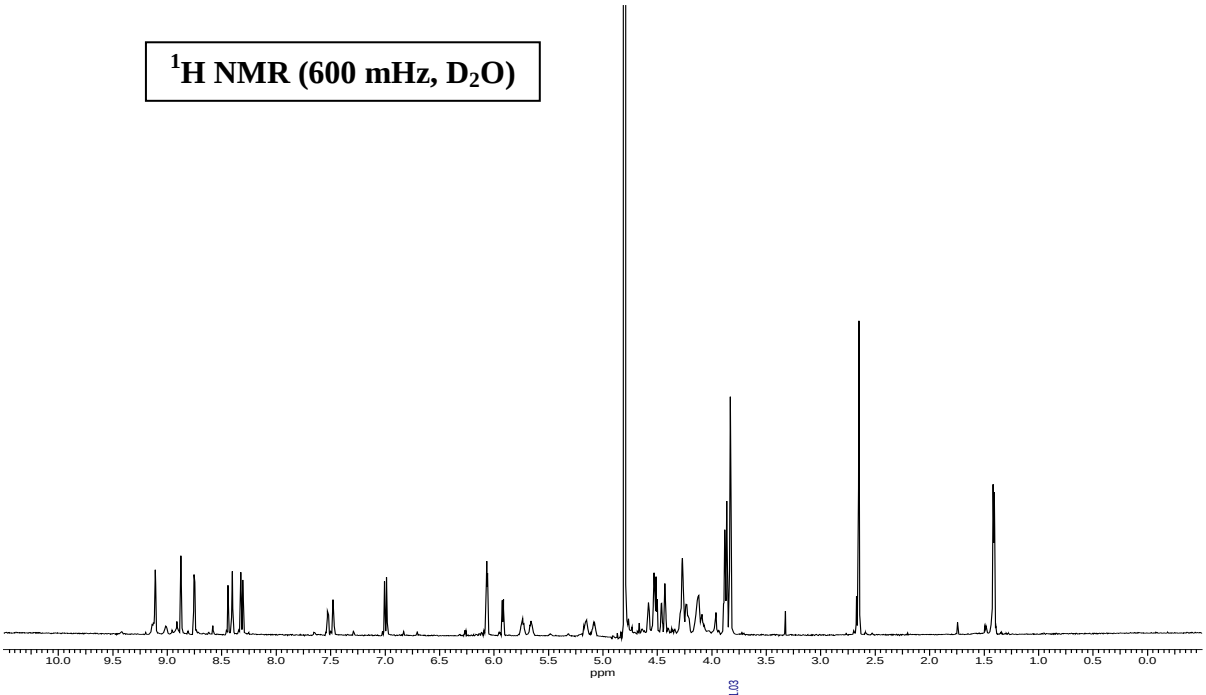


Figure S10. Structure, ^{1}H NMR, ^{31}P NMR, HPLC trace, and HRMS of caged 5-thiomethyl-NAADP



^{1}H NMR (600 mHz, D_2O)



^{31}P NMR (162 mHz, D_2O)

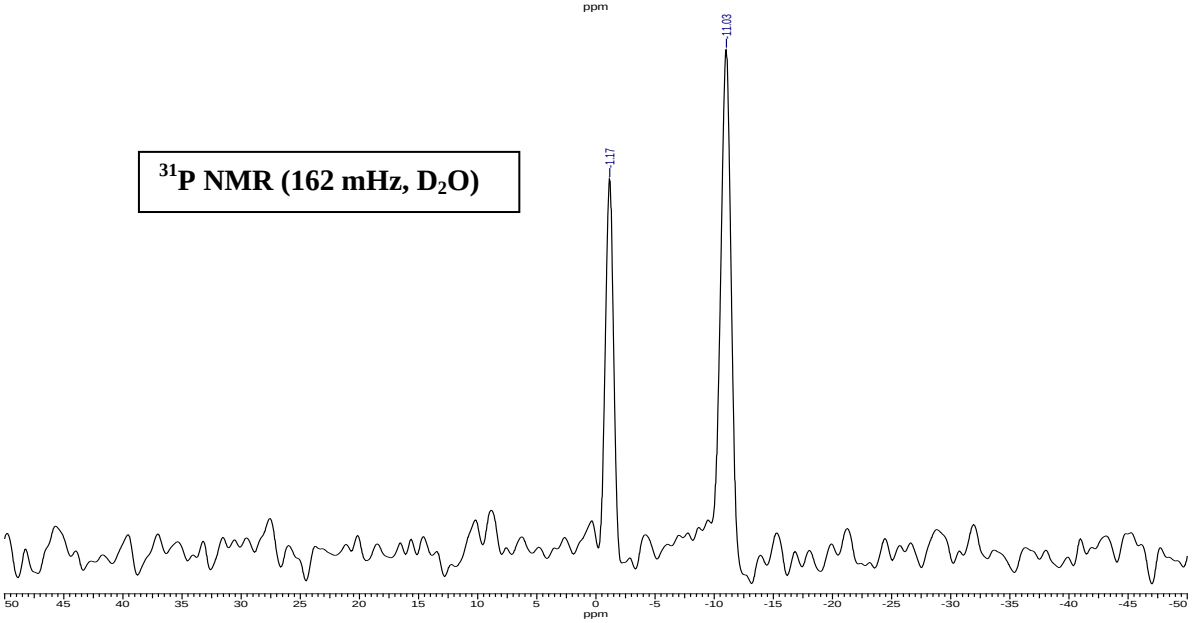


Figure S10 continued