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Electronic Supplementary Information

Probing lysine mono-methylation in histone H3 tail peptides with an abiotic receptor coupled to a non-plasmonic resonator

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Table of Contents

General Methods

^{1}H and ^{31}P NMR spectra were recorded on a Bruker Avance 400 (400 MHz) NMR spectrometer. All ^{1}H chemical shifts (δ) were reported in parts per million (ppm) relative to proton resonances resulting from incomplete deuteration of NMR solvents. All ^{31}P chemical shifts (δ) were reported in parts per million (ppm) relative to external 85% H_3PO_3 set at 0 ppm. All titrations were performed by adding progressive aliquots of a $1 \bullet 10^{-3}$ M solution of the peptides in CD_3OD to a $1 \bullet 10^{-3}$ M solution (1 mL) of **Tiiii[C_3H_7, CH_3, Ph]** in CD_3OD.

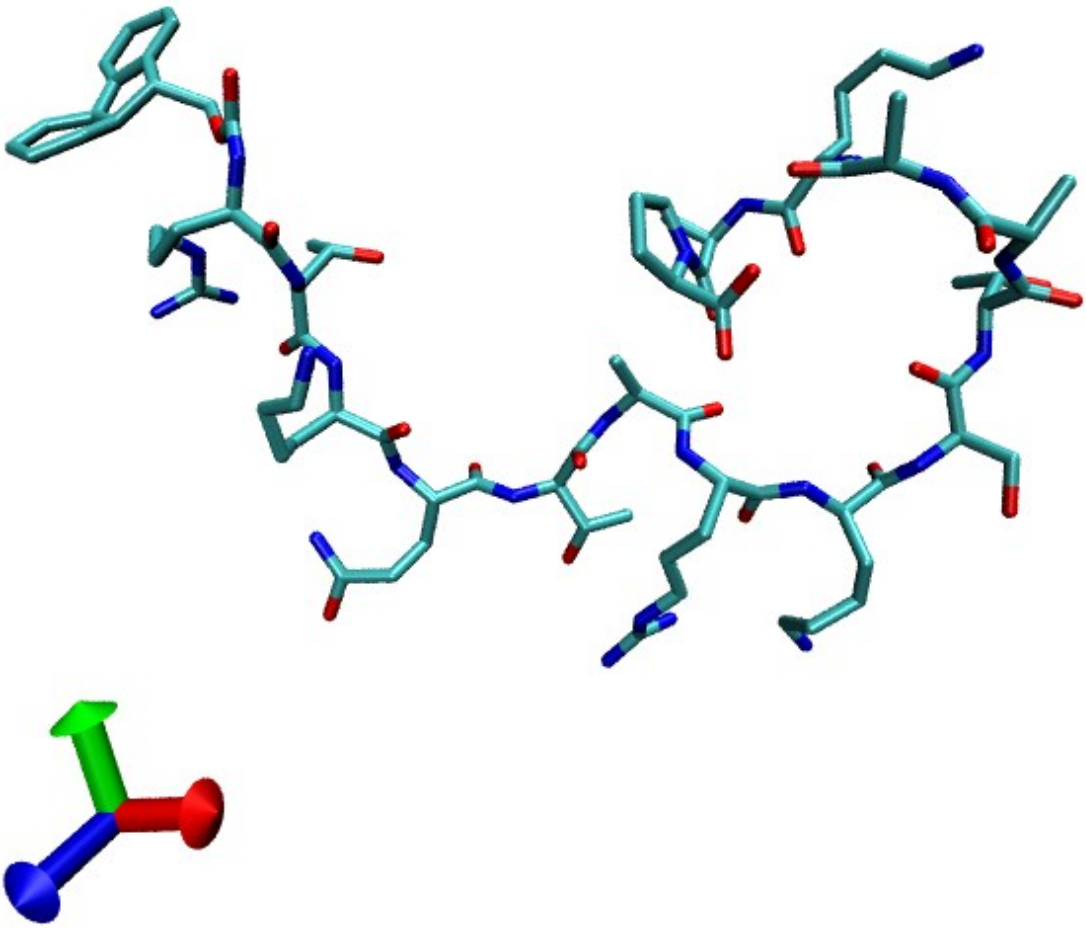

Figure S1. Simulated structure of reference H3 histone PC in ethanol

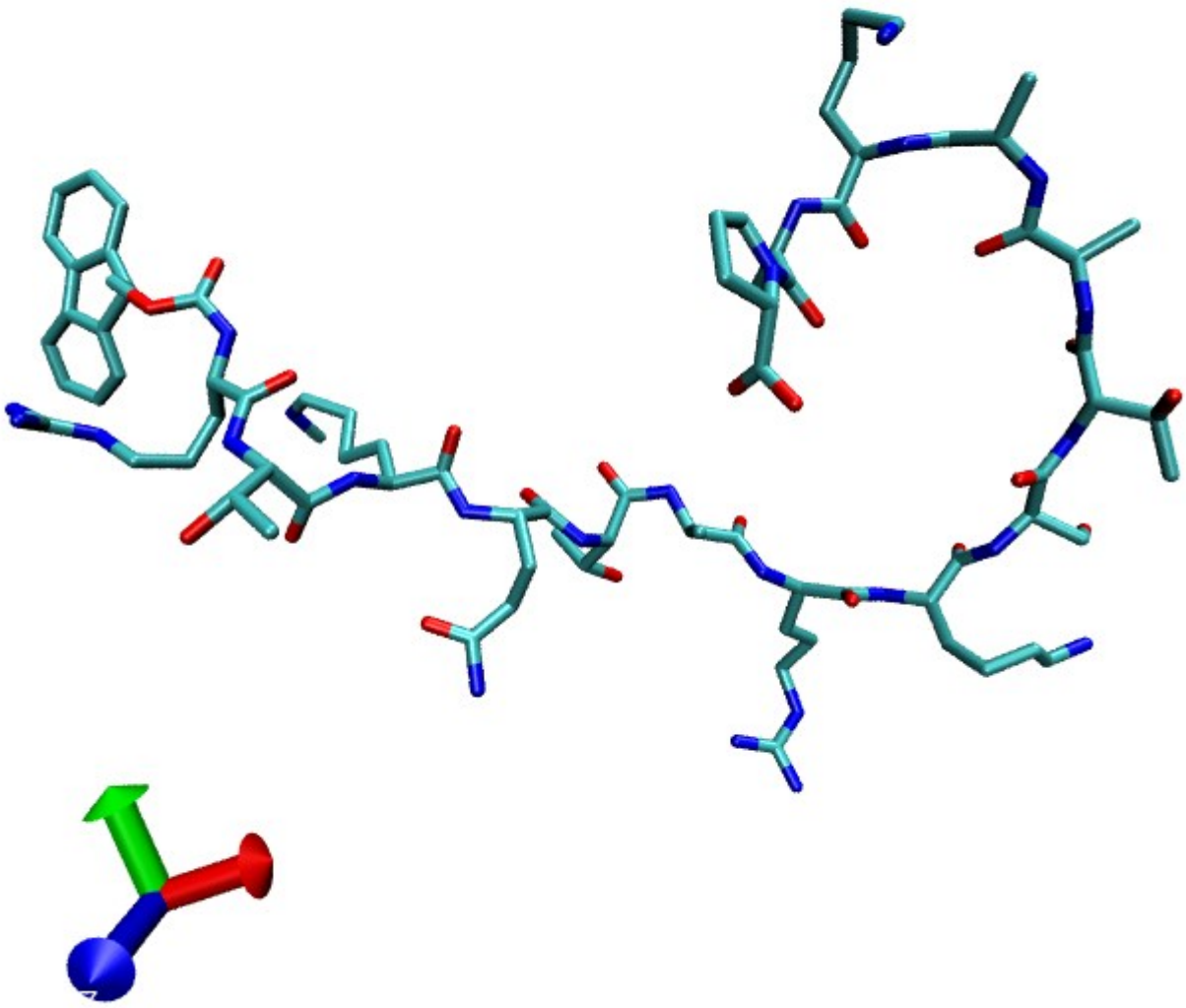

Figure S2. Simulated structure of Lys4 mono-methylated H3 histone P1 in ethanol

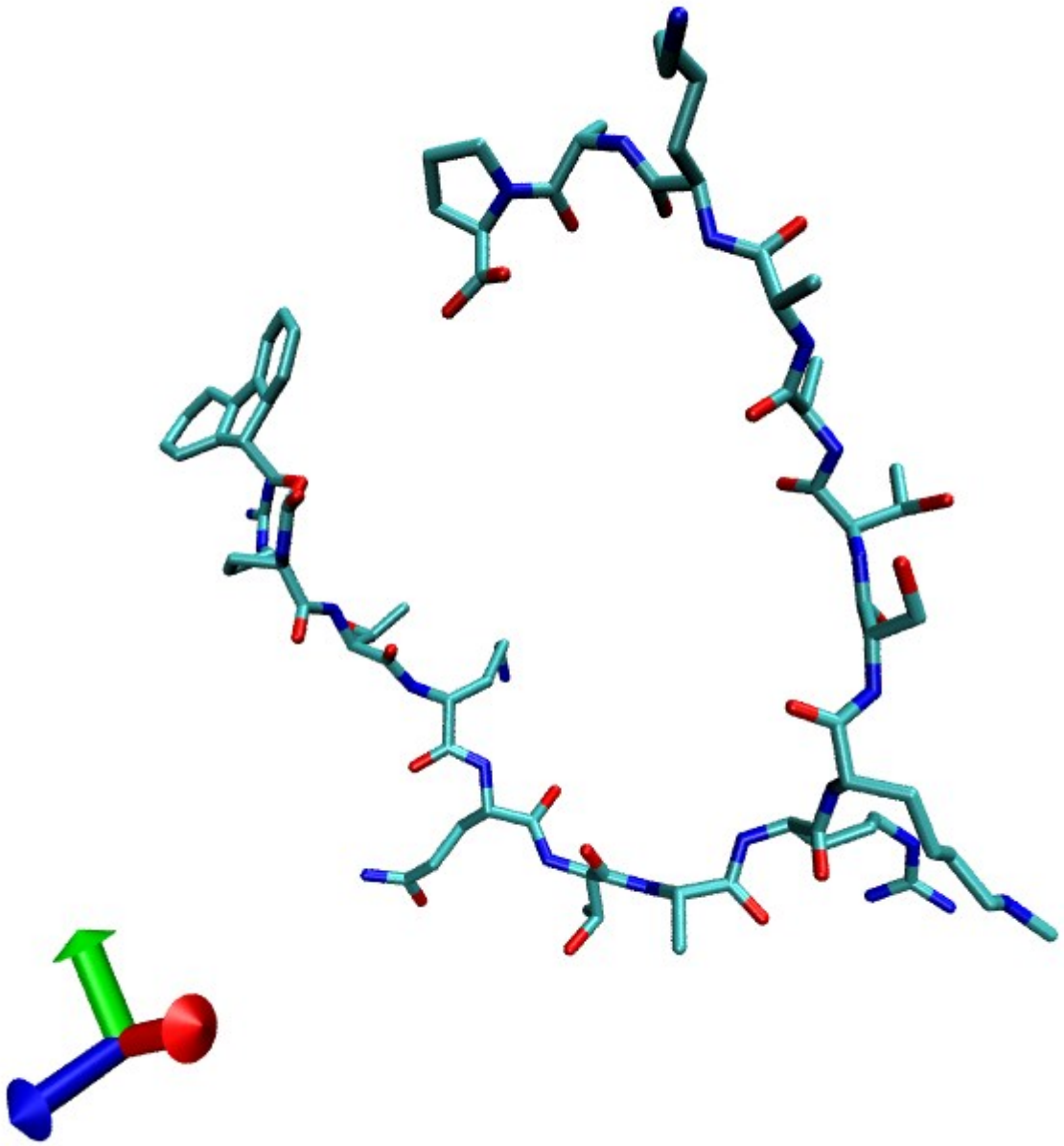

Figure S3. Simulated structure of Lys9 mono-methylated H3 histone P2 in ethanol

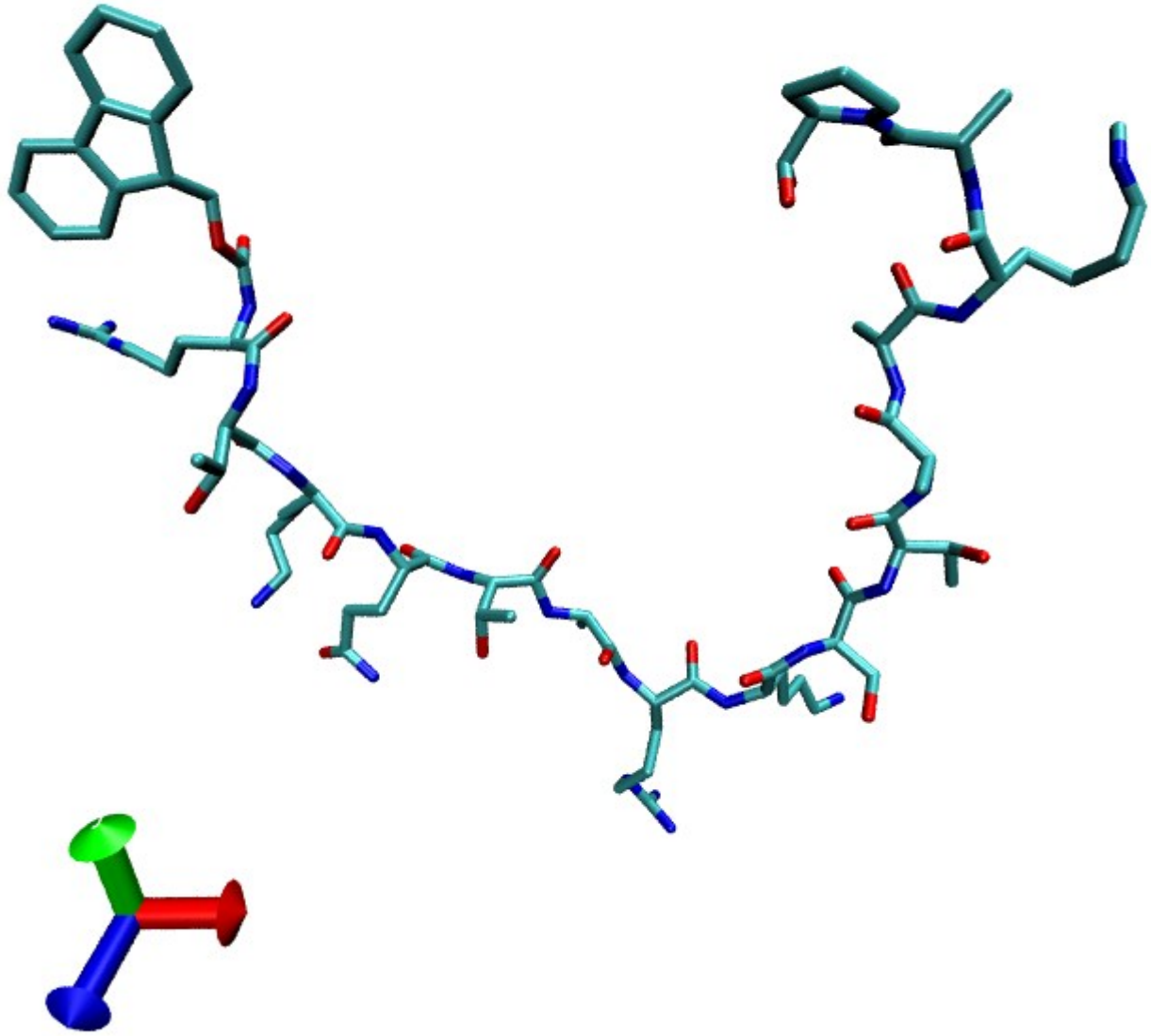

Figure S4. Simulated structure of Lys14 mono-methylated H3 histone P3 in ethanol

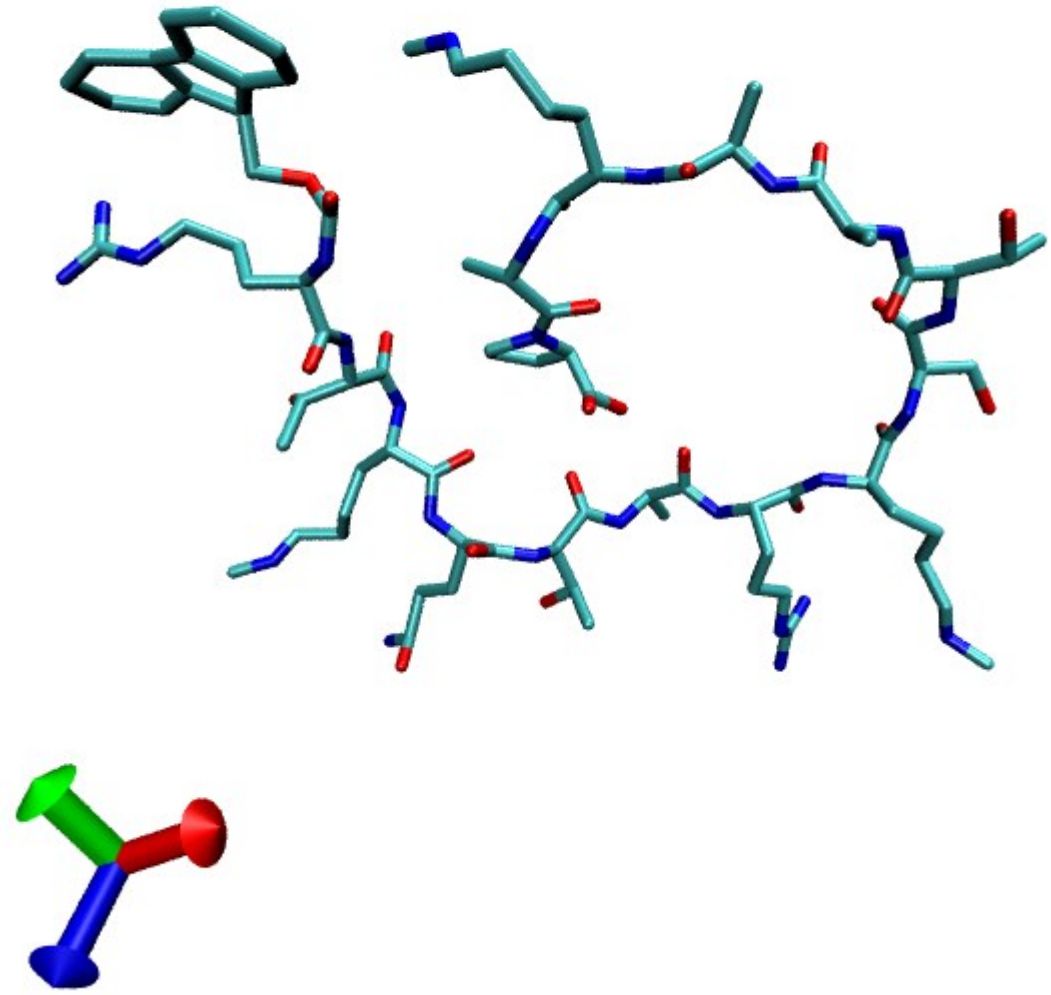

Figure S5. Simulated structure of Lys4, Lys9, Lys14 mono-methylated H3 histone P123 in ethanol

Titration in Methanol-d_4 via ^{31}P and ^{1}H-NMR

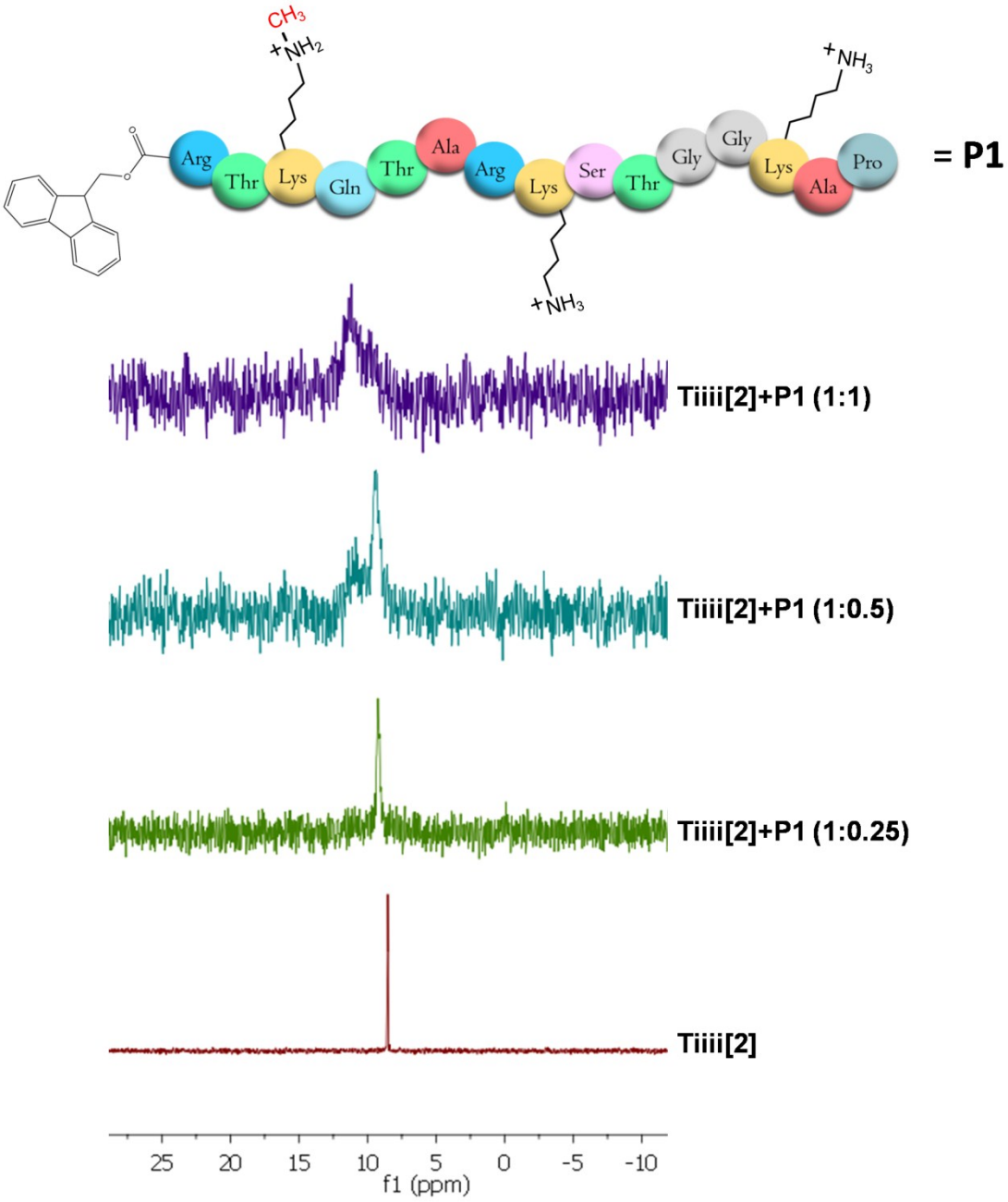

Figure S6. ^{31}P NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P1** added (green and blue spectra) and the 1:1 complex (violet spectrum). $\Delta_{P=O}$ = -2.65ppm.

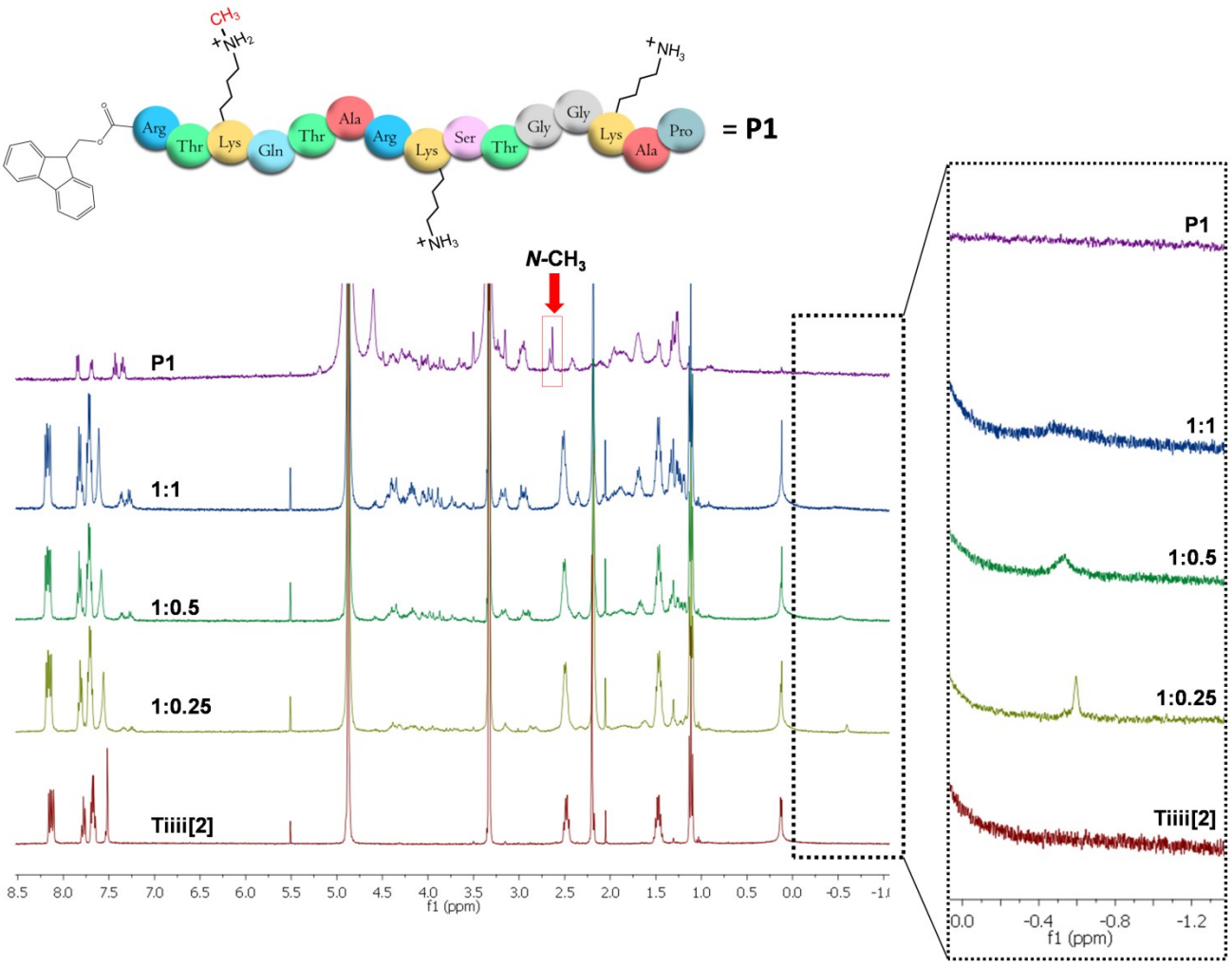

Figure S7. ^{1}H NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P1** added (green spectra), the 1:1 complex (blue spectrum) and the free **P1** (violet spectrum). $\Delta_{N\text{-}CH3} = 3.25$ppm

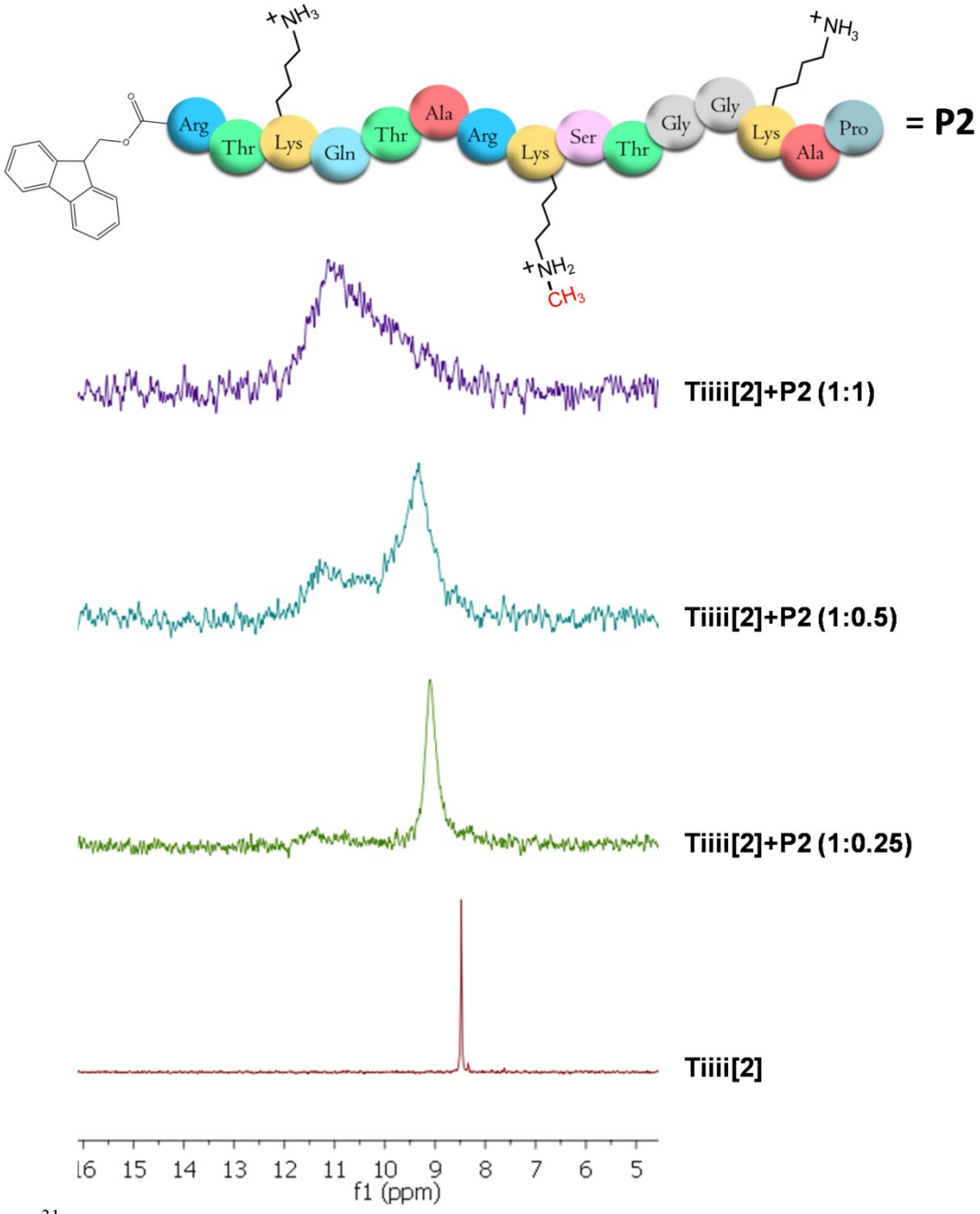

Figure S8. ^{31}P NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P2** added (green and blue spectra) and the 1:1 complex (violet spectrum). $\Delta_{P=O}$ = -2.66ppm

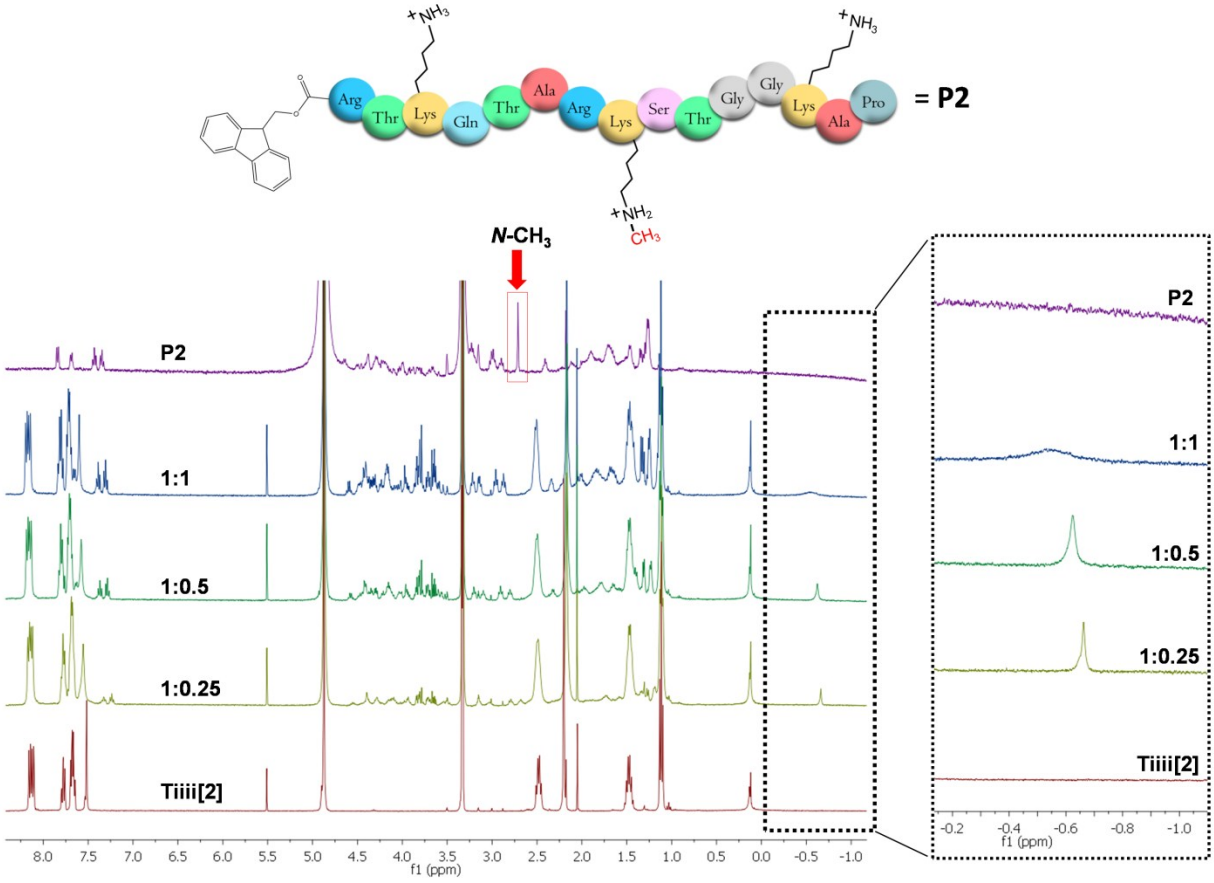

Figure S9. ^{1}H NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P2** added (green spectra), the 1:1 complex (blue spectrum) and the free **P2** (violet spectrum). $\Delta_{N\text{-}CH_3} = 3.37$ppm

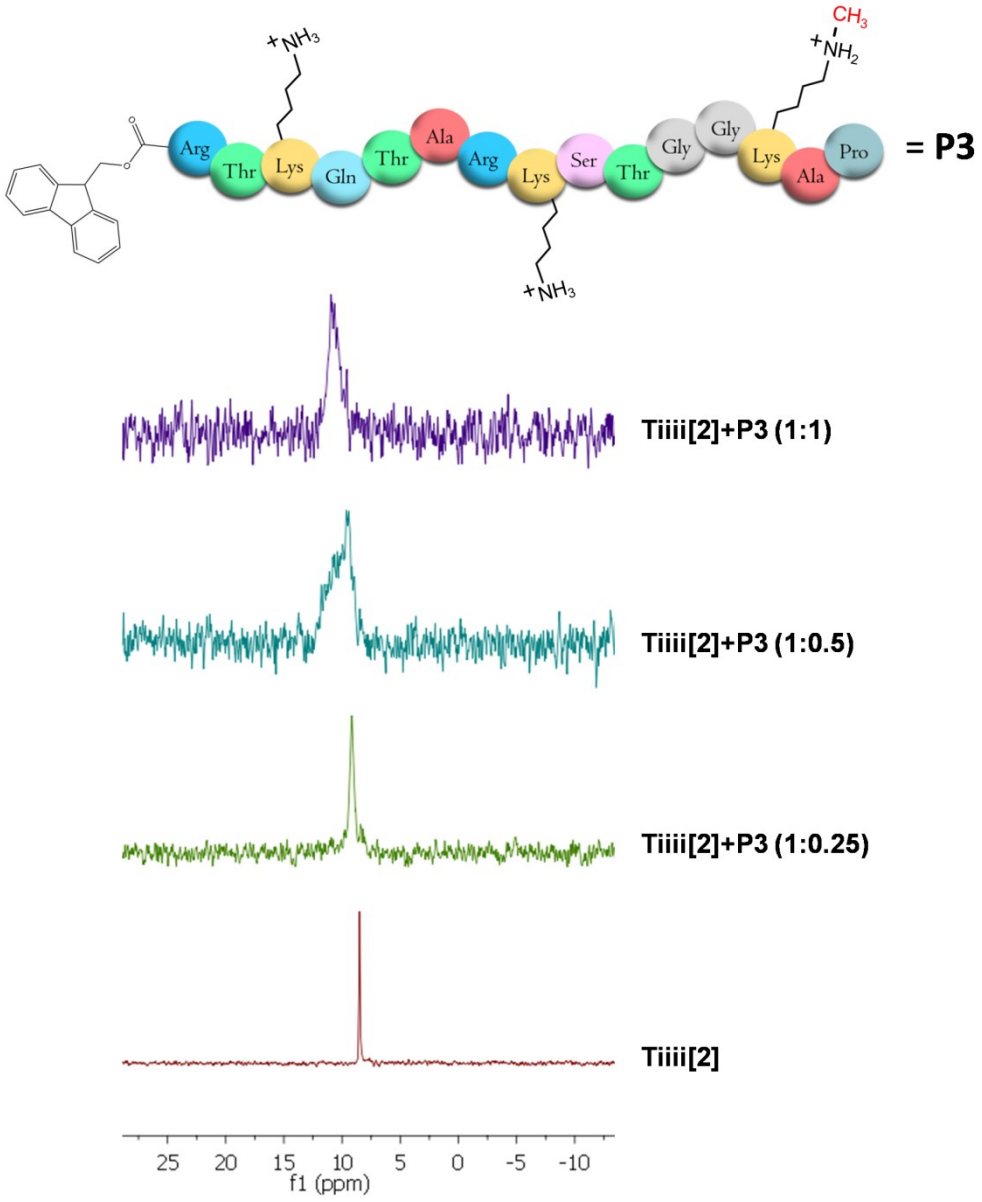

Figure S10. ^{31}P NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P3** added (green and blue spectra) and the 1:1 complex (violet spectrum). $\Delta_{P=O}$ = -2.41ppm

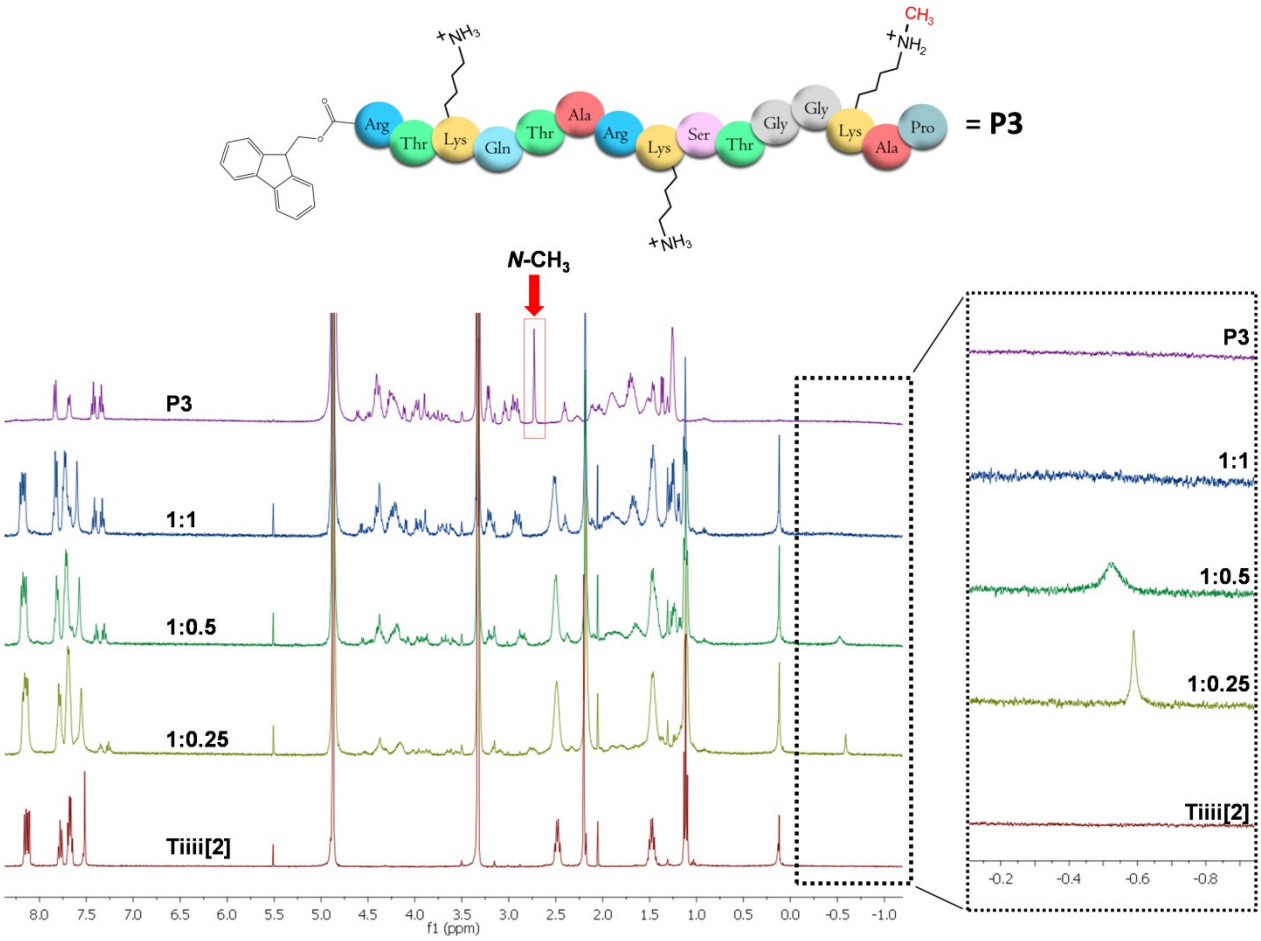

Figure S11. ^{1}H NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P3** added (green spectra), the 1:1 complex (blue spectrum) and the free **P3** (violet spectrum). $\Delta_{N\text{-}CH_3} = 3.32$ppm

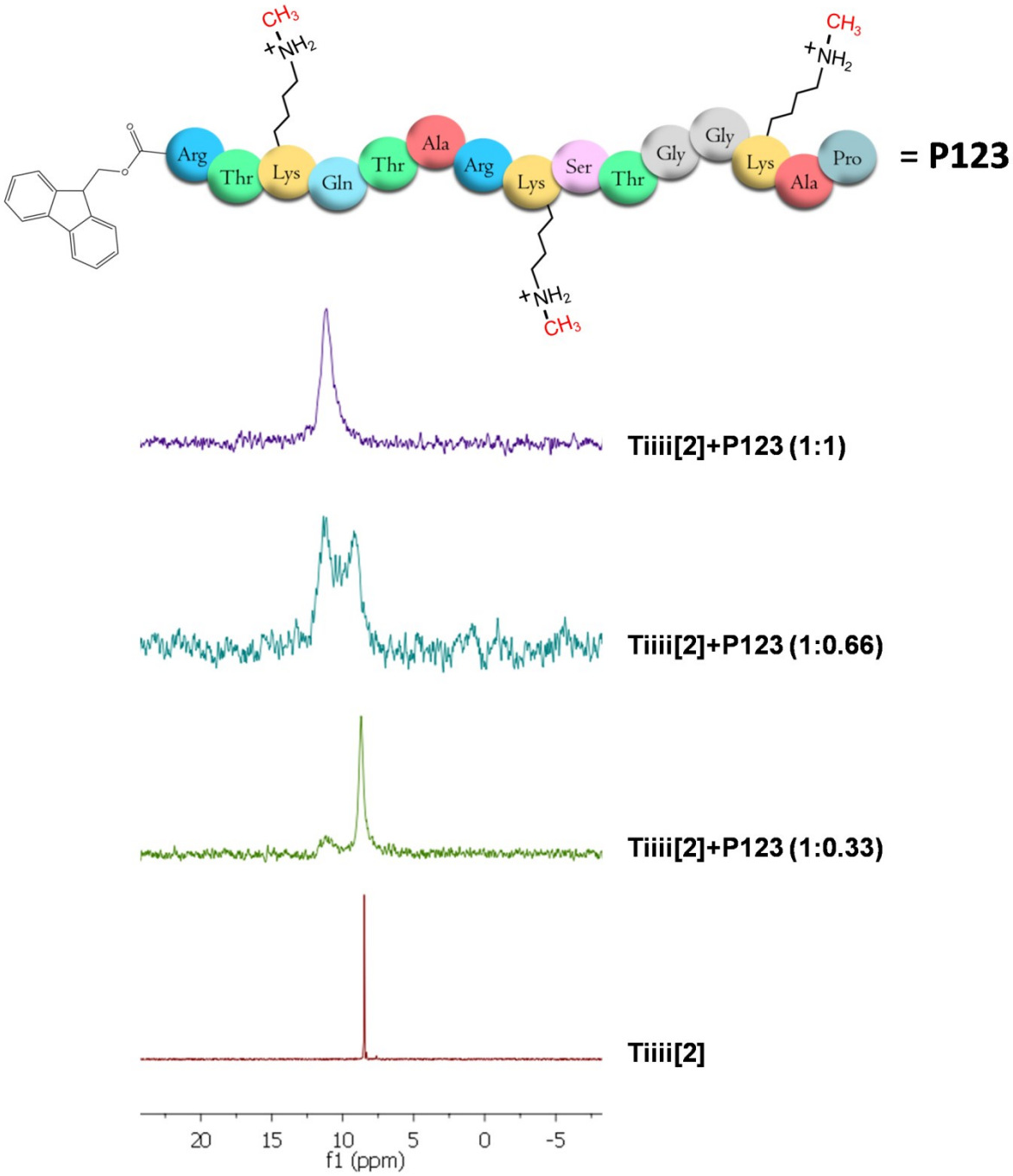

Figure S12. ^{31}P NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P123** added (green and blue spectra) and the 1:1 complex (violet spectrum). $\Delta_{P=O}$ = -2.92ppm

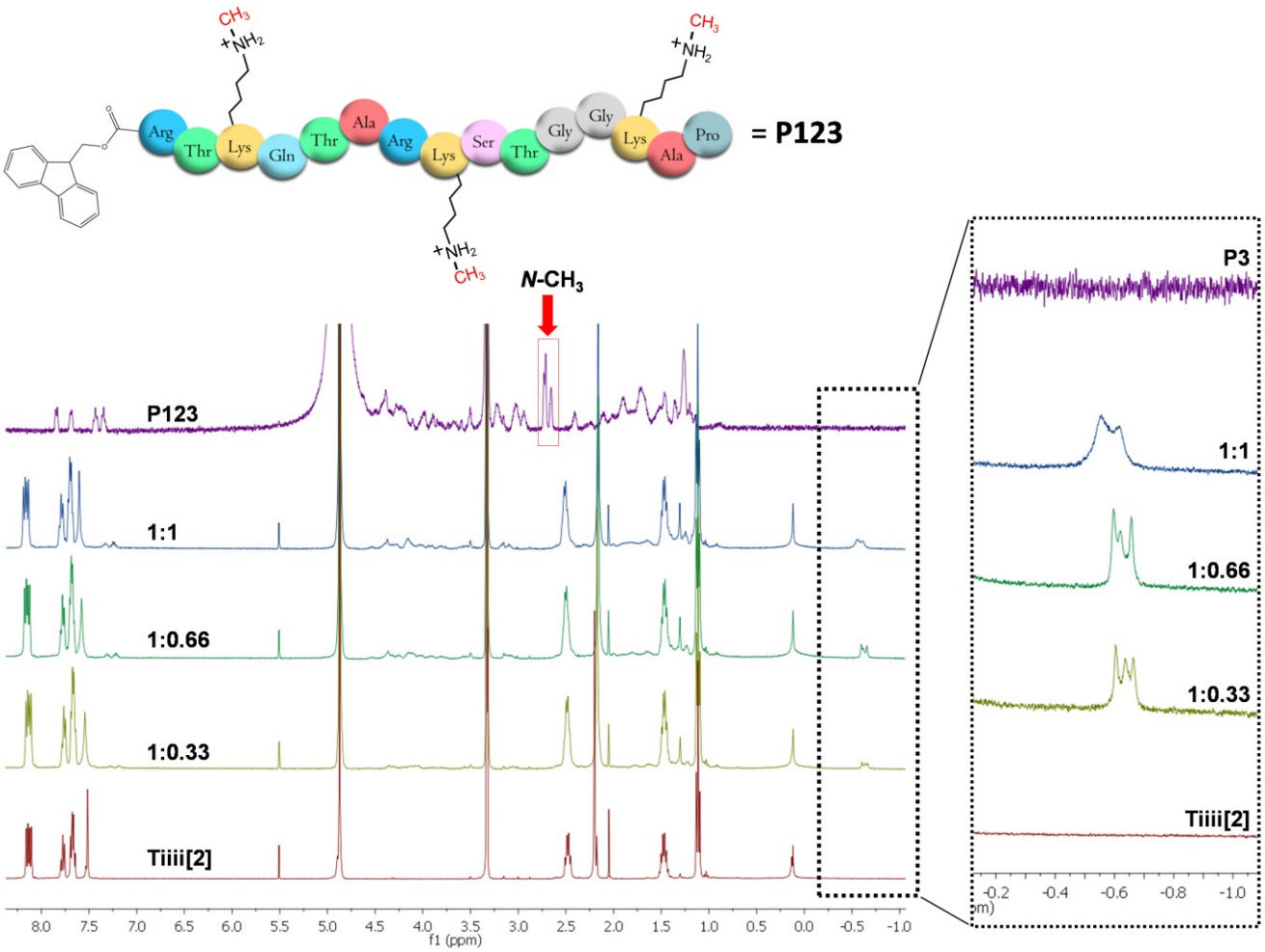

Figure S13. ^{1}H NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **P123** added (green spectra), the 1:1 complex (blue spectrum) and the free **P123** (violet spectrum). $\Delta_{N\text{-}CH_3}$ = 3.33ppm

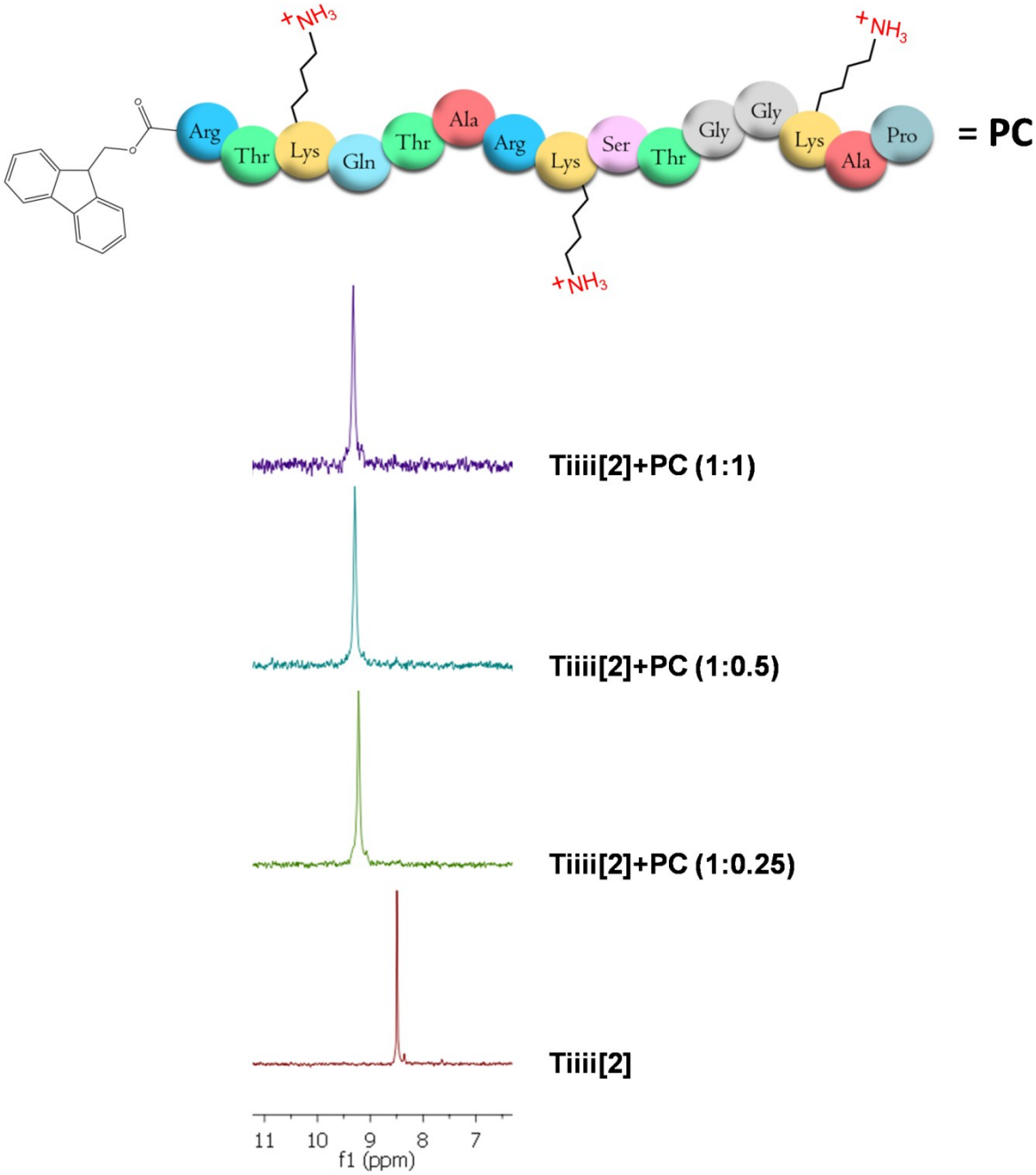

Figure S14. ^{31}P NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **PC** added (green and blue spectra) and the 1:1 complex (violet spectrum). $\Delta_{P=O}$ = -0.83ppm

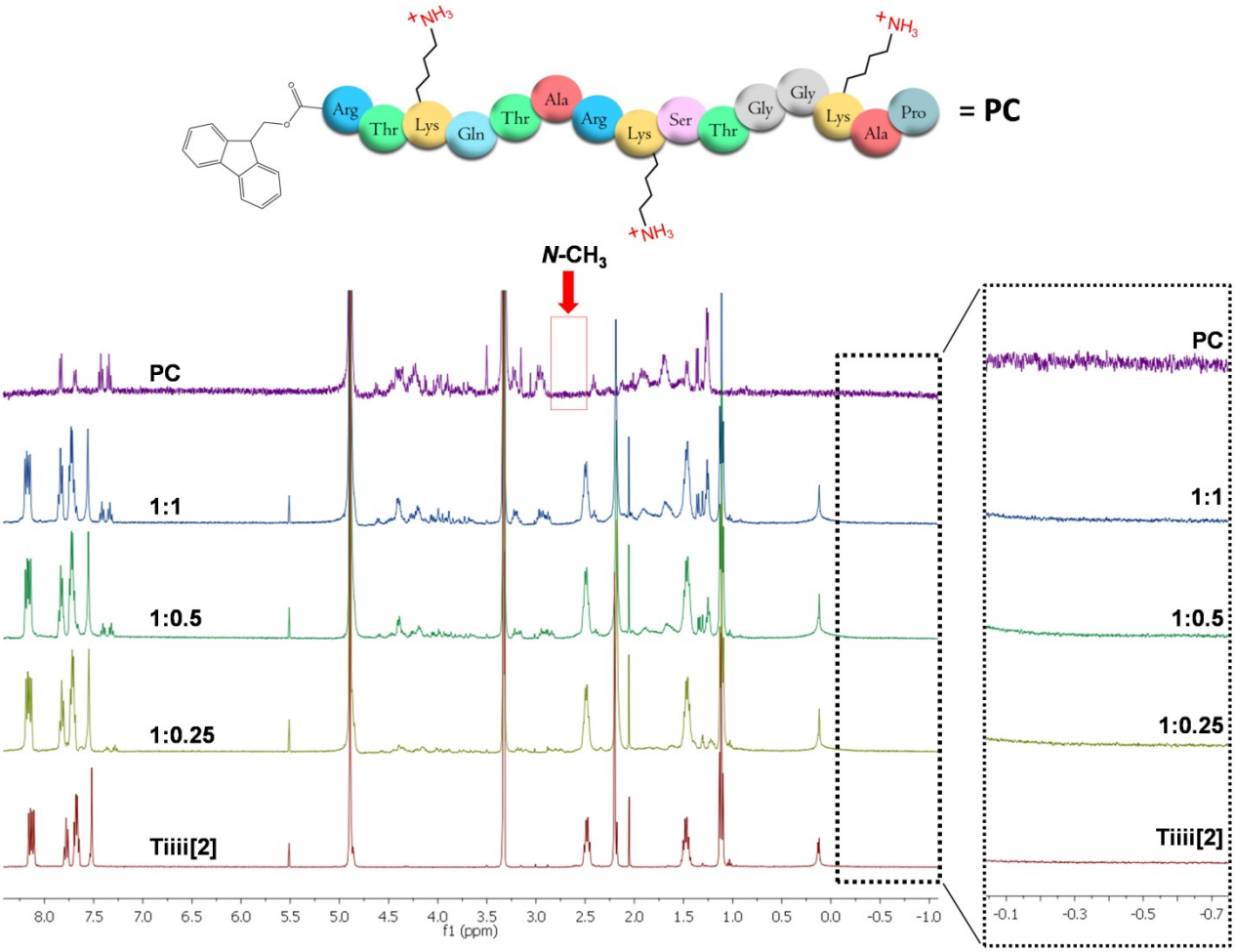

Figure S15. ^{1}H NMR spectra (400 MHz, CD_3OD, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (**Tiiii[2],** red spectrum), 0.25eq. and 0.5 eq. of **PC** added (green spectra), the 1:1 complex (blue spectrum) and the free **PC** (violet spectrum).