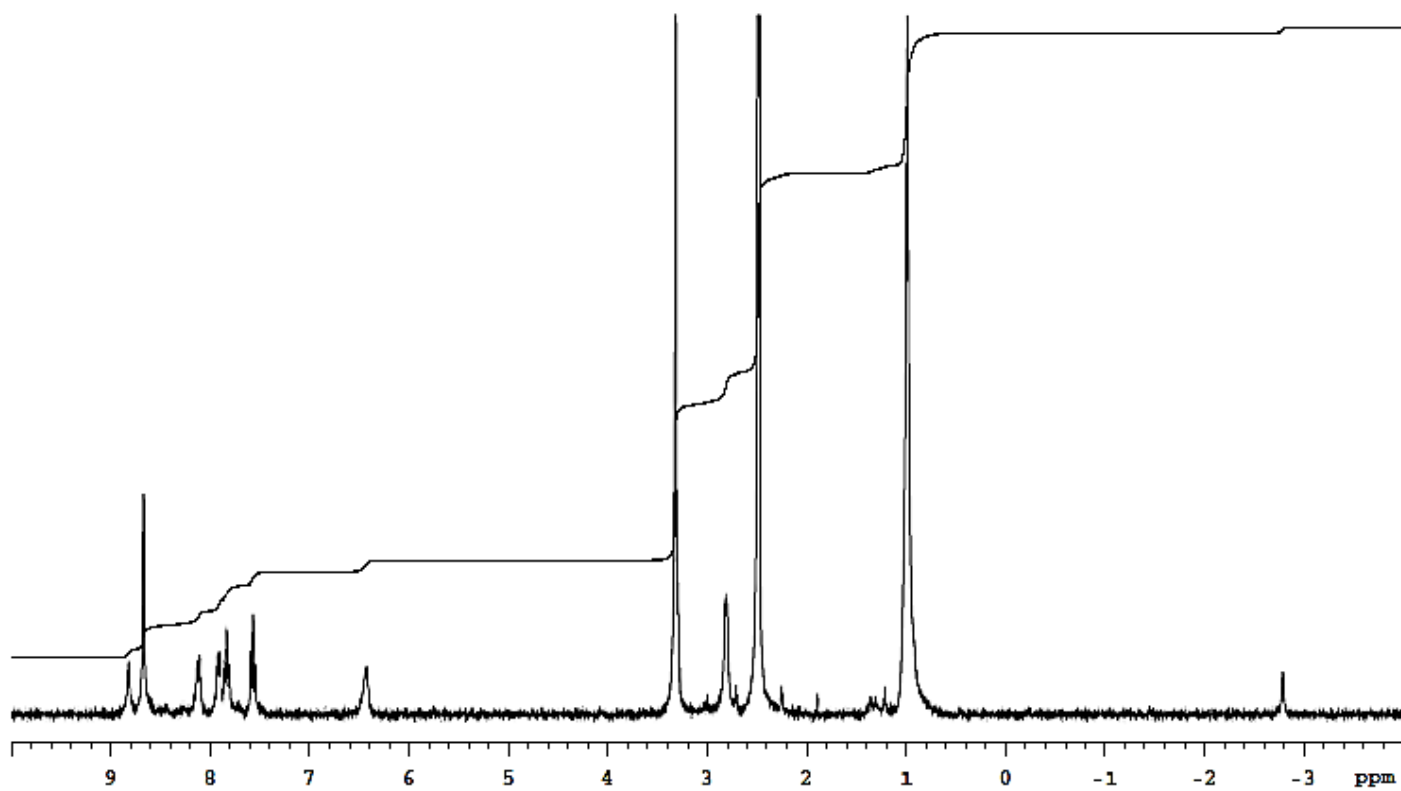


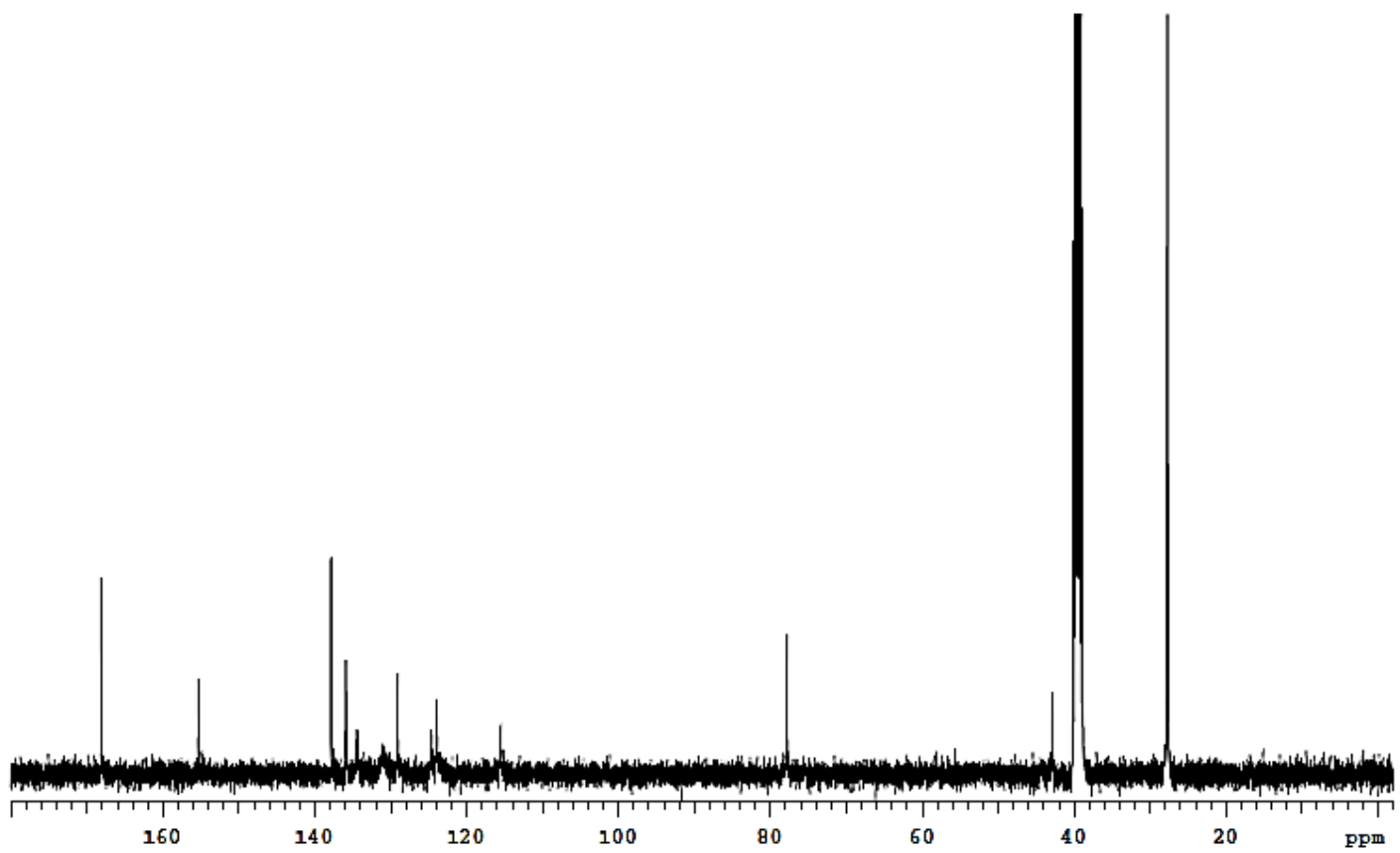
SI for “Developing a Targeting System for Bacterial Membranes: Measuring Receptor-Phosphatidylglycerol Interactions with ^1H NMR, ITC, and Fluorescence Correlation Spectroscopy

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S-Index	Pages S1
S-Figure 1: ^1H NMR of 3	Page S2
S-Figure 2: ^{13}C NMR of 3	Page S3
S-Figure 3: HRMS of 3	Page S4
S-Figure 4: ^1H NMR of 4a	Page S5
S-Figure 5: ^{13}C NMR of 4a	Page S6
S-Figure 6: ^{19}F NMR of 4a	Page S7
S-Figure 7: HRMS of 4a	Page S8
S-Figure 8: ^1H NMR of 4b	Page S9
S-Figure 9: ^{13}C NMR of 4b	Page S10
S-Figure 10: ^{19}F NMR of 4b	Page S11
S-Figure 11: ^{31}P NMR of 4b	Page S12
S-Figure 12: ^{31}P NMR of NH_4PF_6	Page S12
S-Figure 13: ESI HRMS of 4b	Page S13
S-Figure 14: Stacked ^1H NMR plot of 4b titrated with TBAPG.....	Page S14
S-Figure 15: Stacked ^1H NMR plot of 4b titrated with TBAPG.....	Page S15
S-Figure 16: Stacked ^1H NMR plot of 4b titrated with TBAH_2PO_4	Page S16
S-Figure 17: Stacked ^1H NMR plot of 4b titrated with TBAH_2PO_4	Page S17
S-Figure 18: ^1H NMR of 4b + CD_3OD	Page S18
S-Figure 19: Stacked ^1H NMR plot of TBAPG titrated with 4b	Page S19
S-Figure 20: Job plot and ^1H NMR binding isotherm of 4b + TBAPG.....	Page S20
S-Figure 21: ITC binding isotherm of 4b + TBAPG	Page S21
S-Figure 22: Bacteria experiment 2 and 4 hr	Page S22
S-Figure 23: Absorption and emission spectrum of 4a	Page S23



S-Figure 1: ^1H NMR of **3** in DMSO-d_6

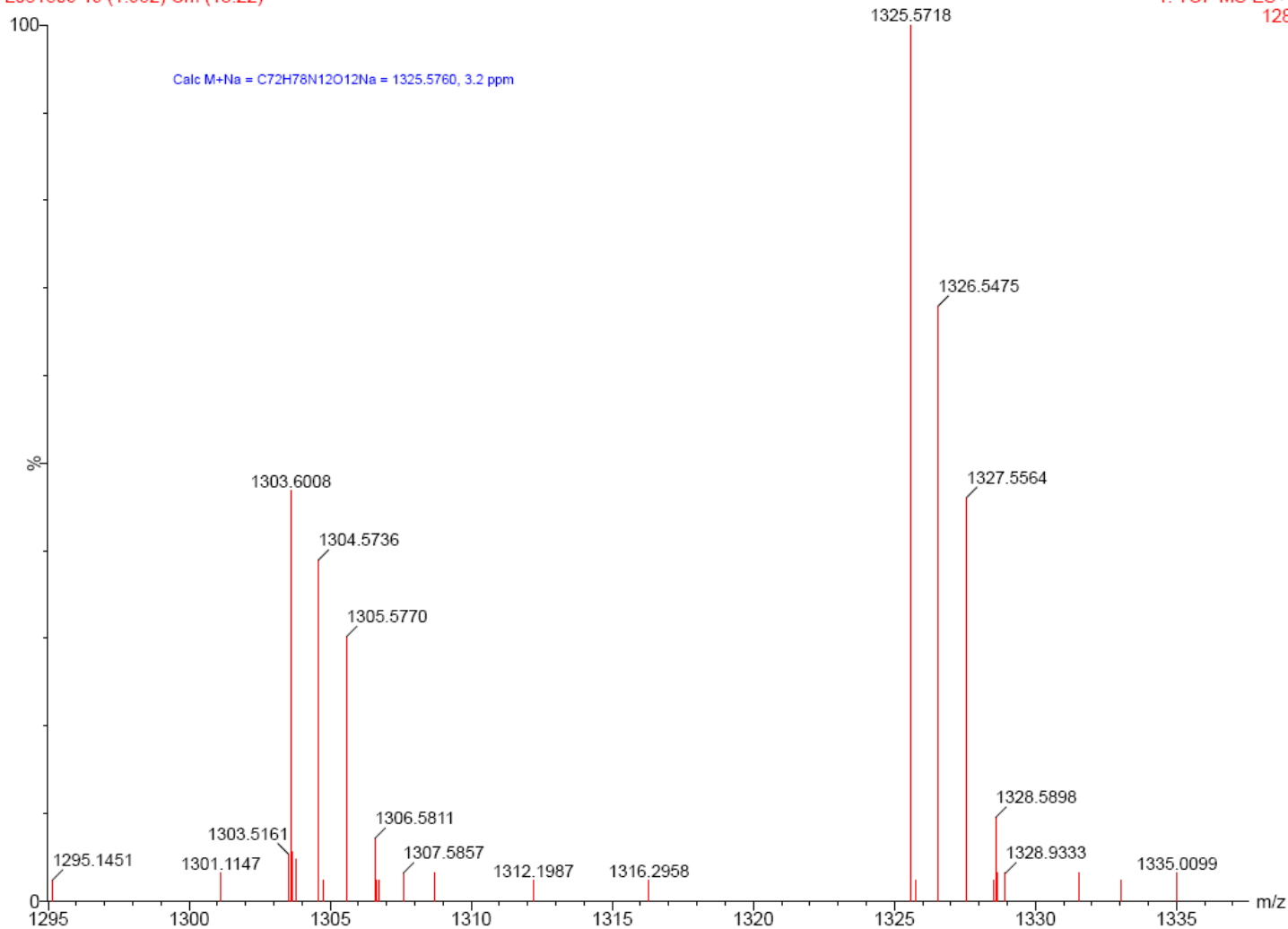


S-Figure 2: ^{13}C NMR of **3** in DMSO-d_6

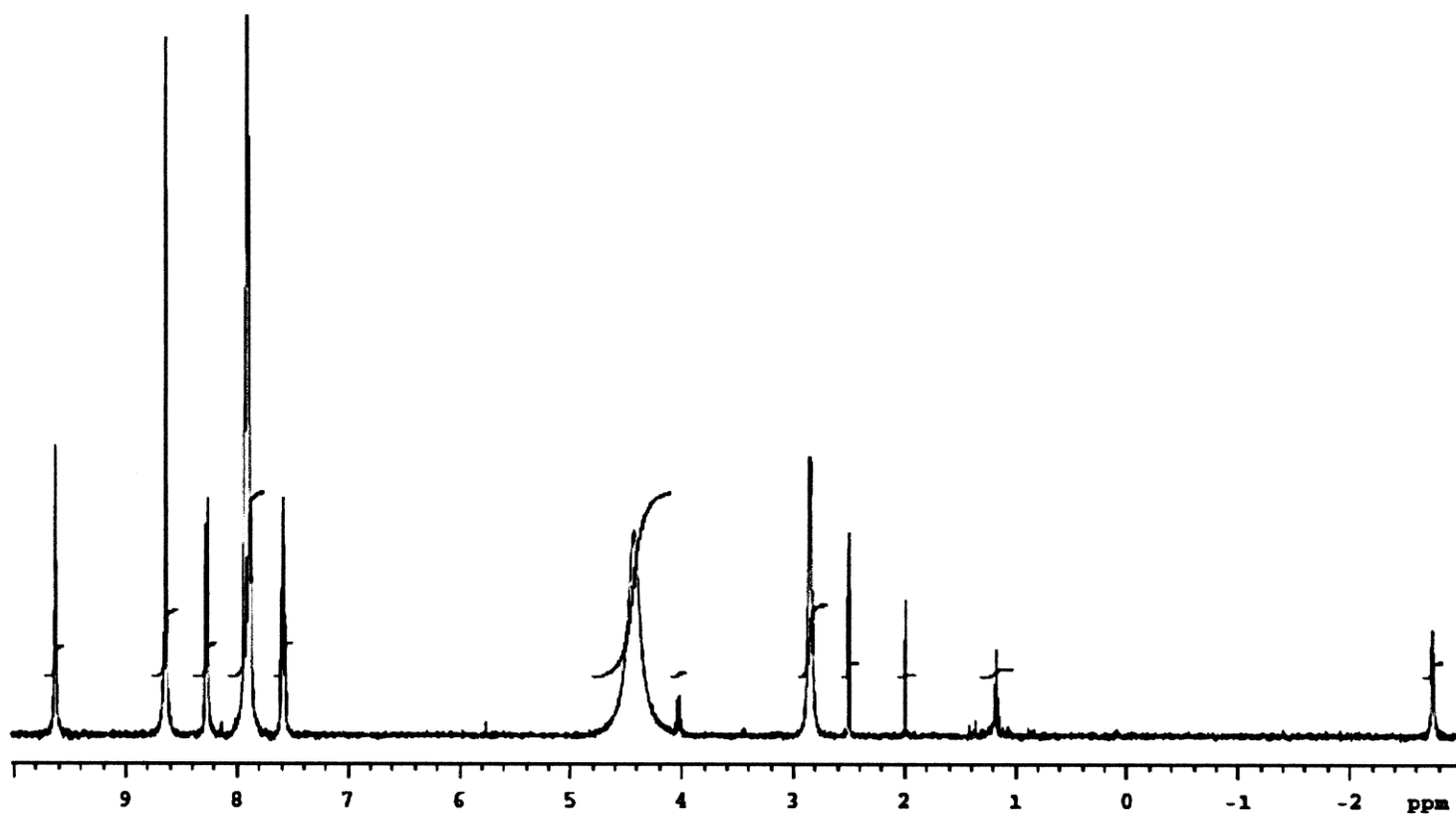
tetra BOC

L081509 19 (1.962) Cm (18:22)

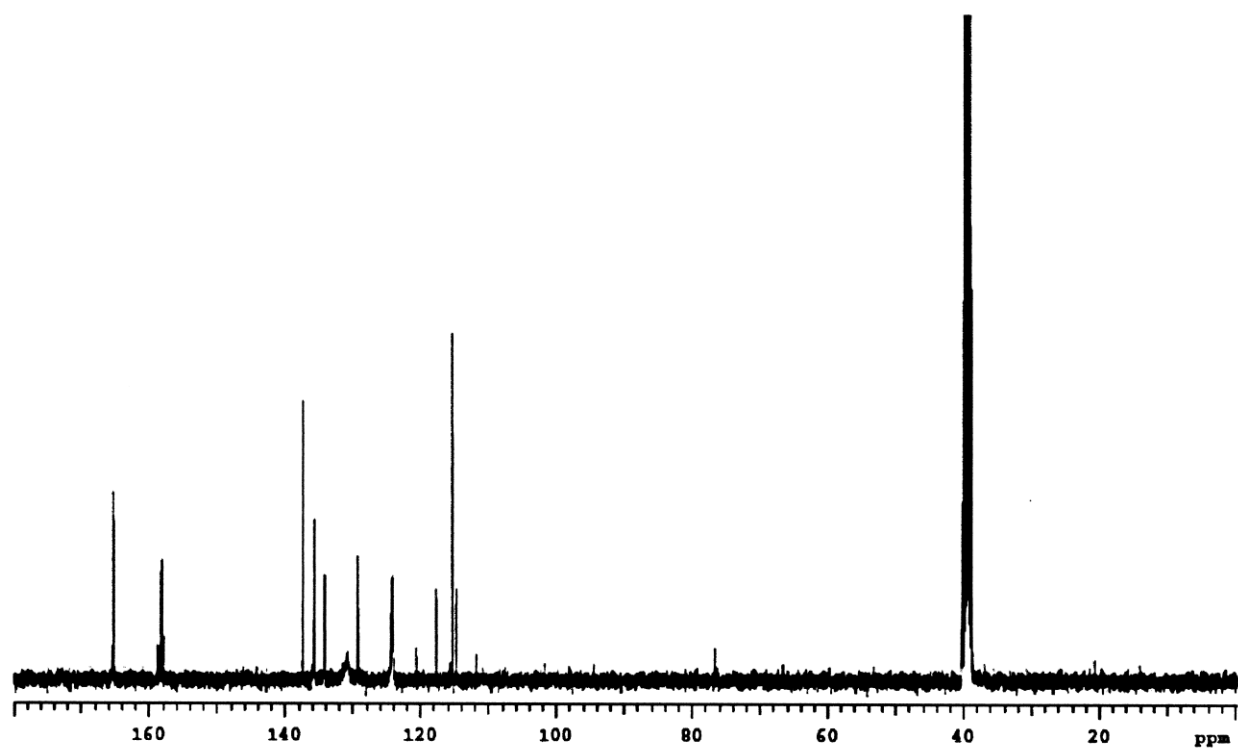
1: TOF MS ES+
128



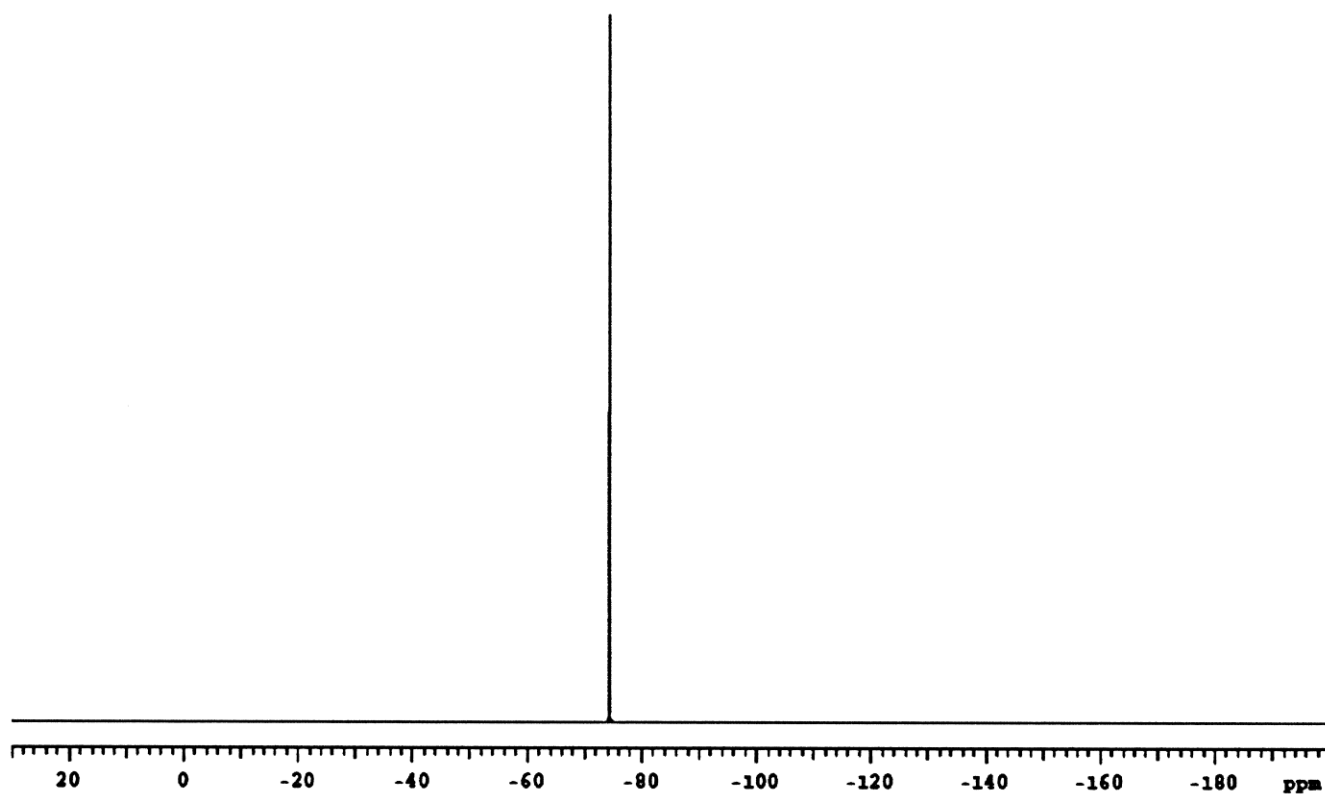
S-Figure 3: HRMS of 3



S-Figure 4: ^1H NMR of **4a** in DMSO-d_6 (resonances at 4.0, 2.0, and 1.15 ppm are ethyl acetate solvent)



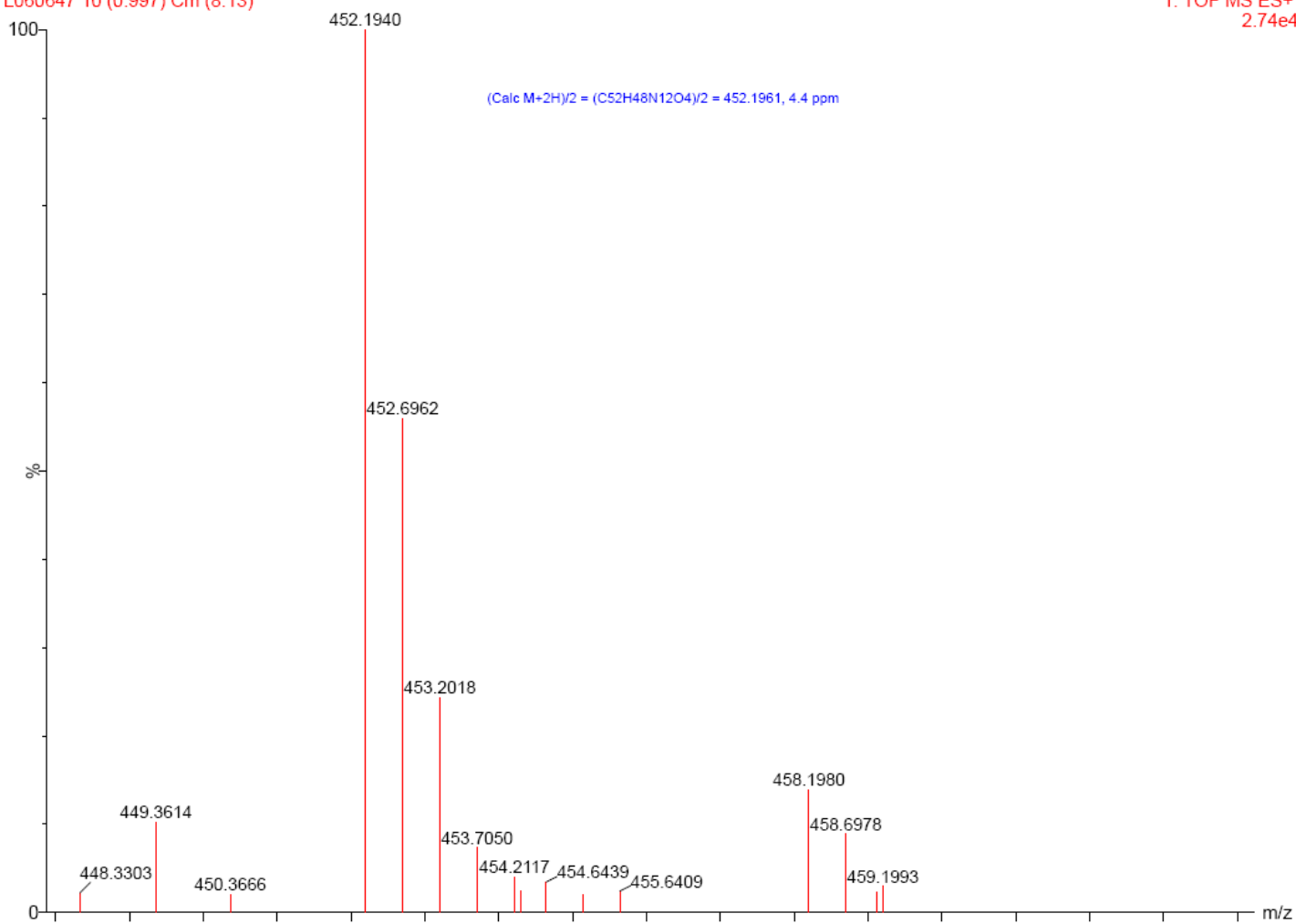
S-Figure 5: ^{13}C NMR of **4a** in DMSO-d_6



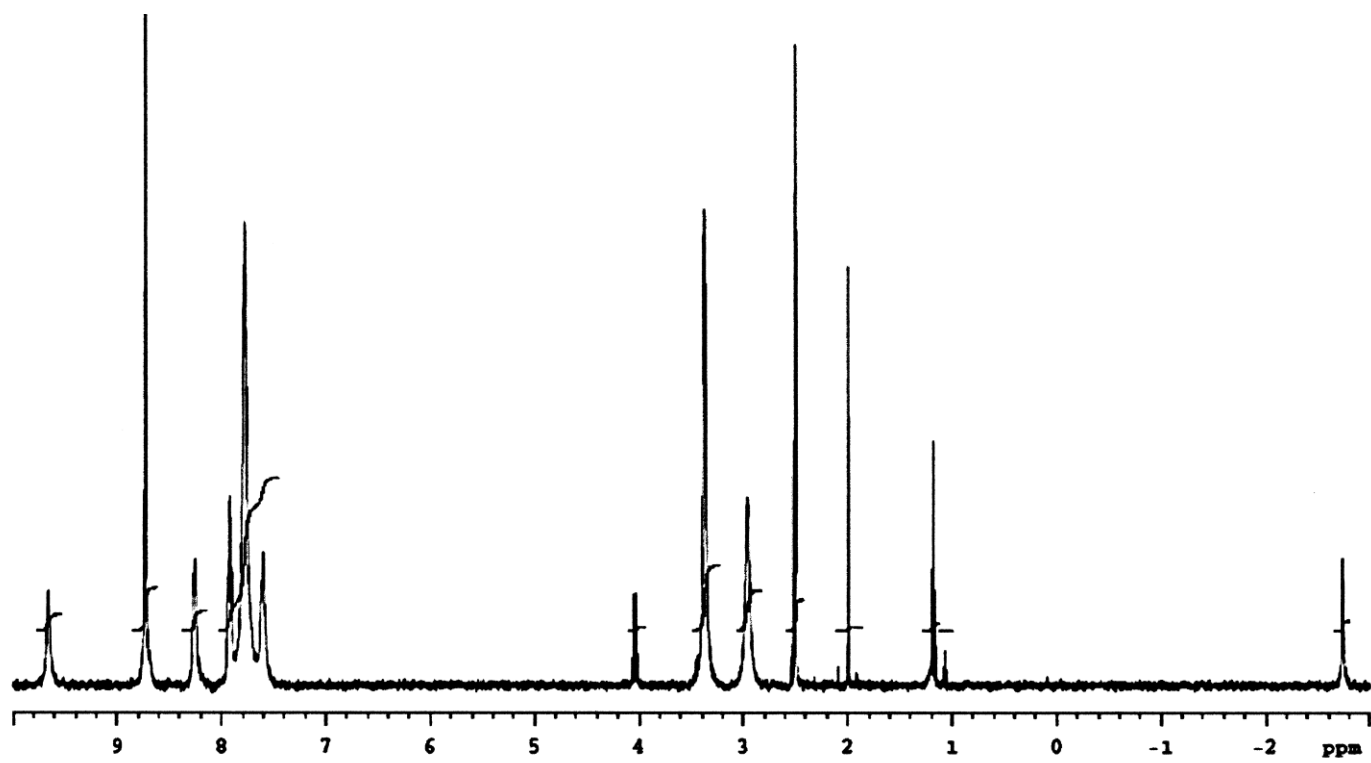
S-Figure 6: ^{19}F NMR of **4a** in DMSO- d_6 (reference is TFA in DMSO- d_6 at -76.55 ppm).

TFA porphyrin in MeOH
L060647 10 (0.997) Cm (8:13)

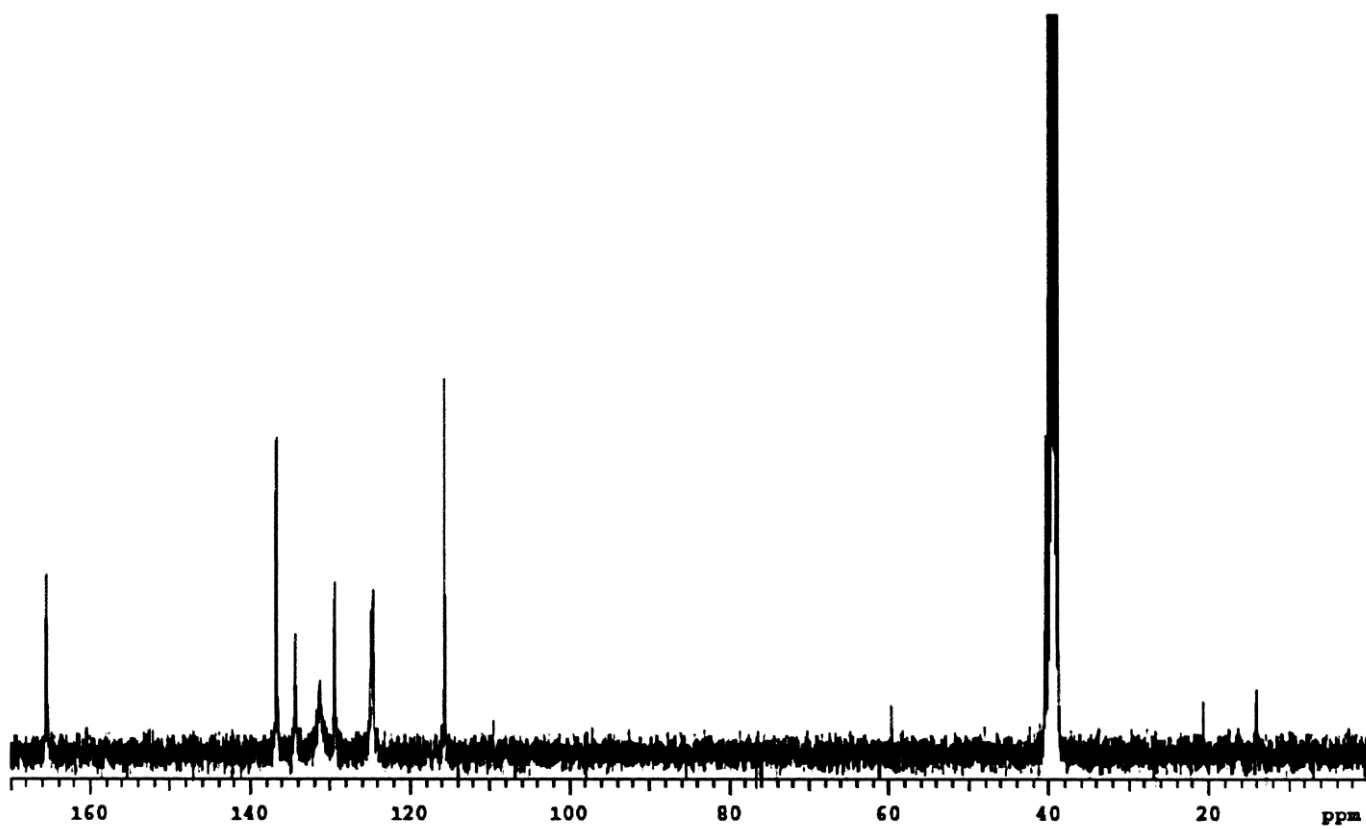
1: TOF MS ES+
2.74e4



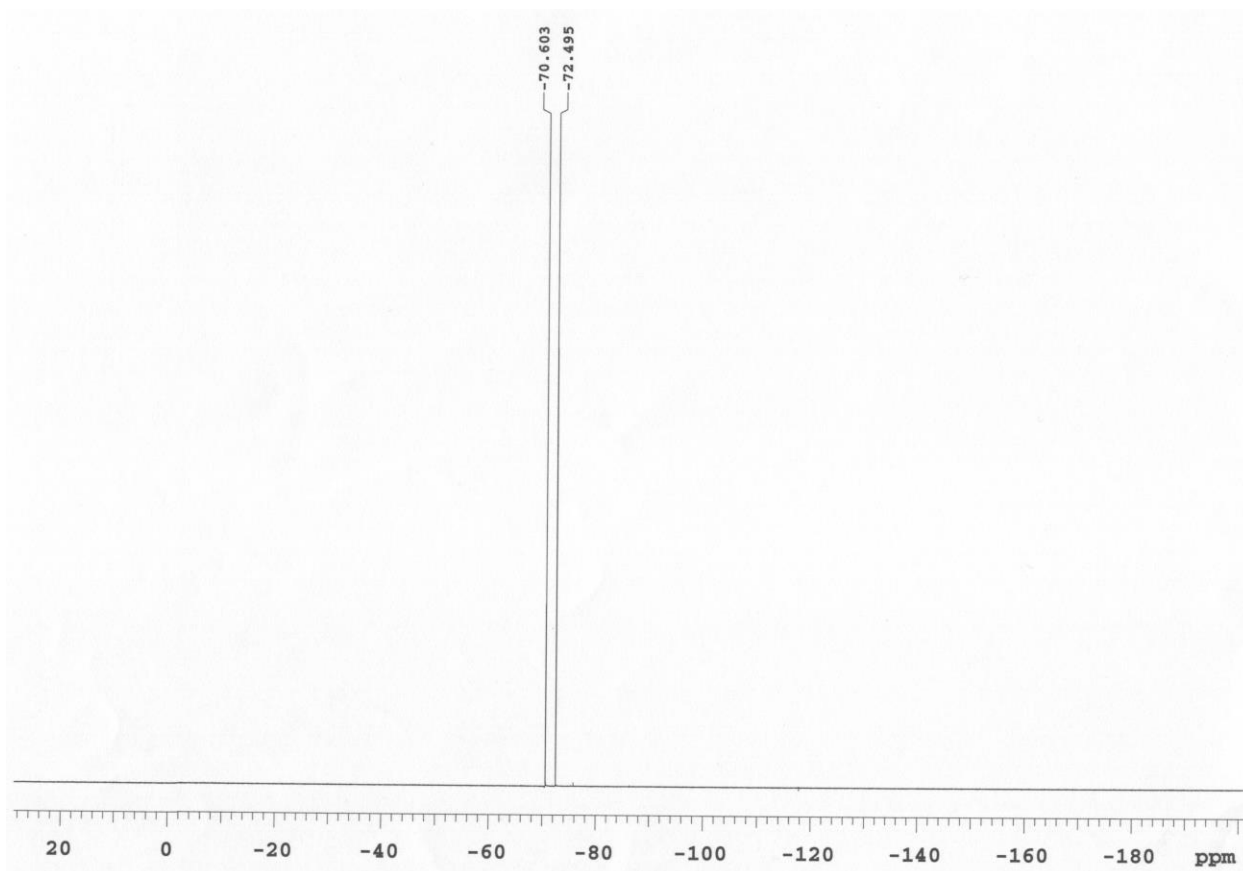
S-Figure 7: ESI HRMS of 4a.



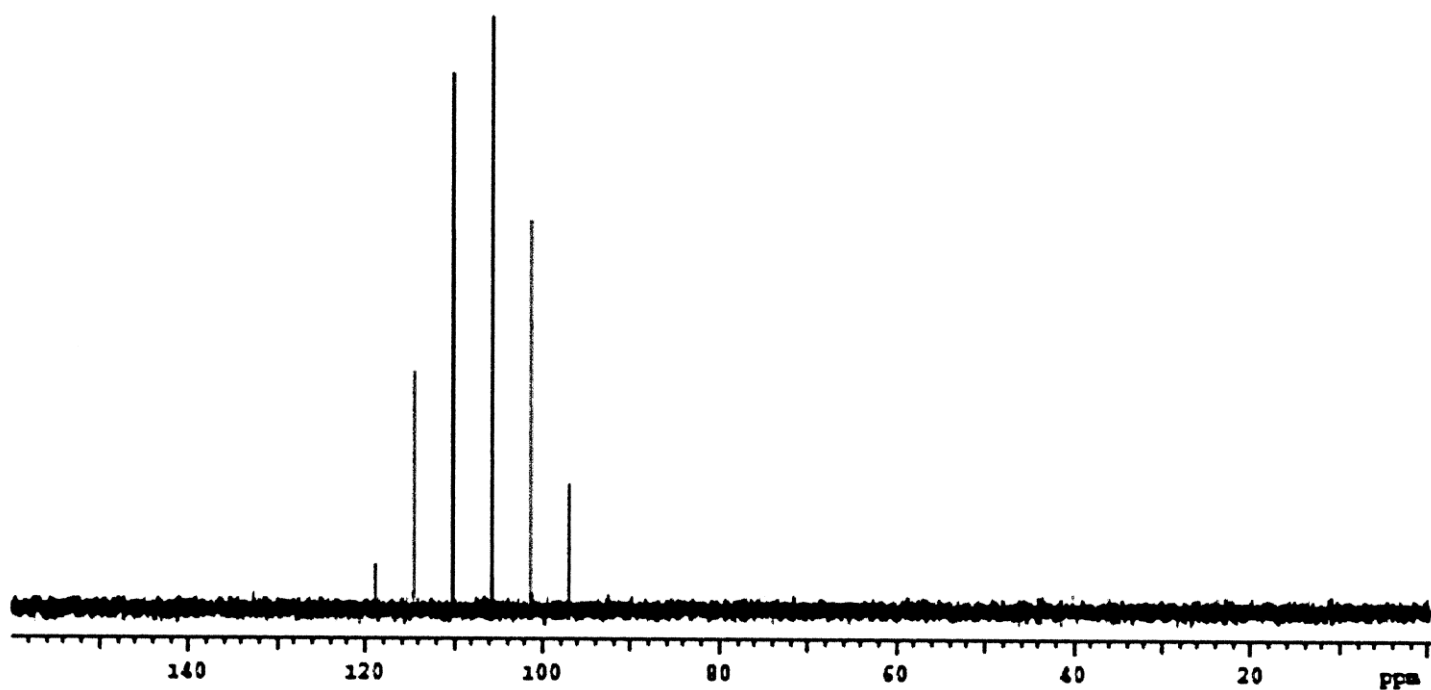
S-Figure 8: ^1H NMR of **4b** in DMSO-d_6 (resonances at 4.0, 2.0, and 1.15 ppm are ethyl acetate solvent)



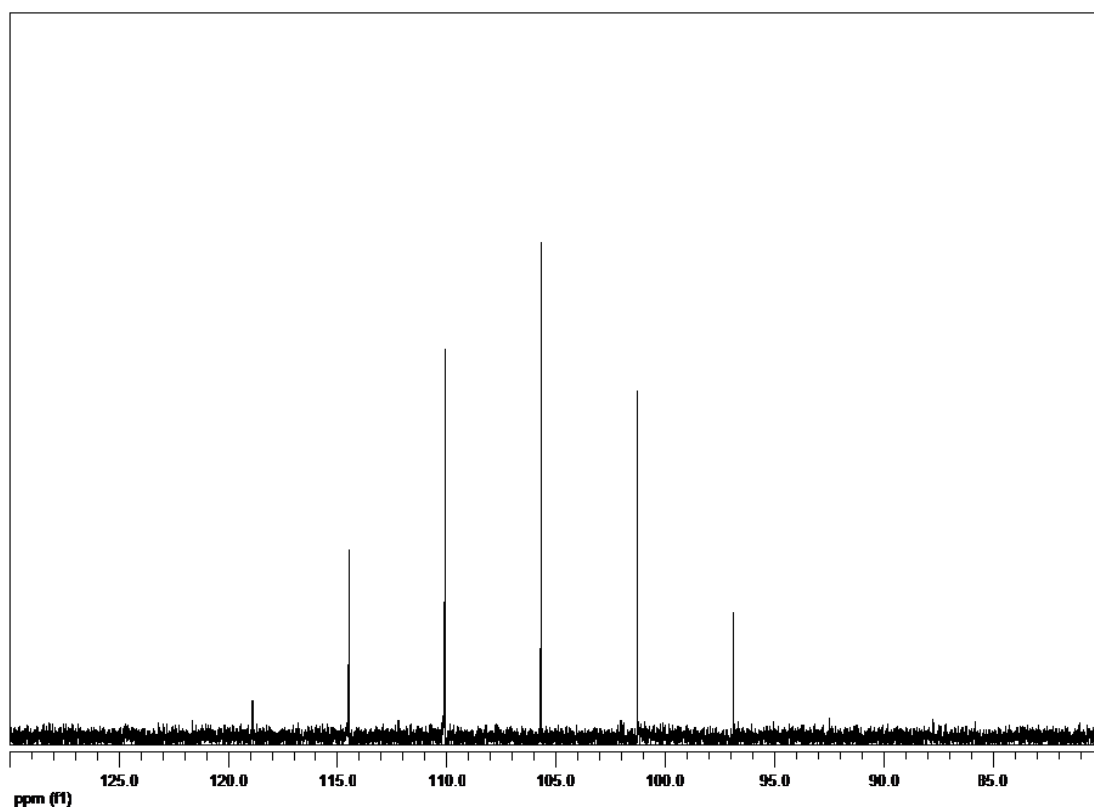
S-Figure 9: ^{13}C NMR of **4b** in DMSO-d_6



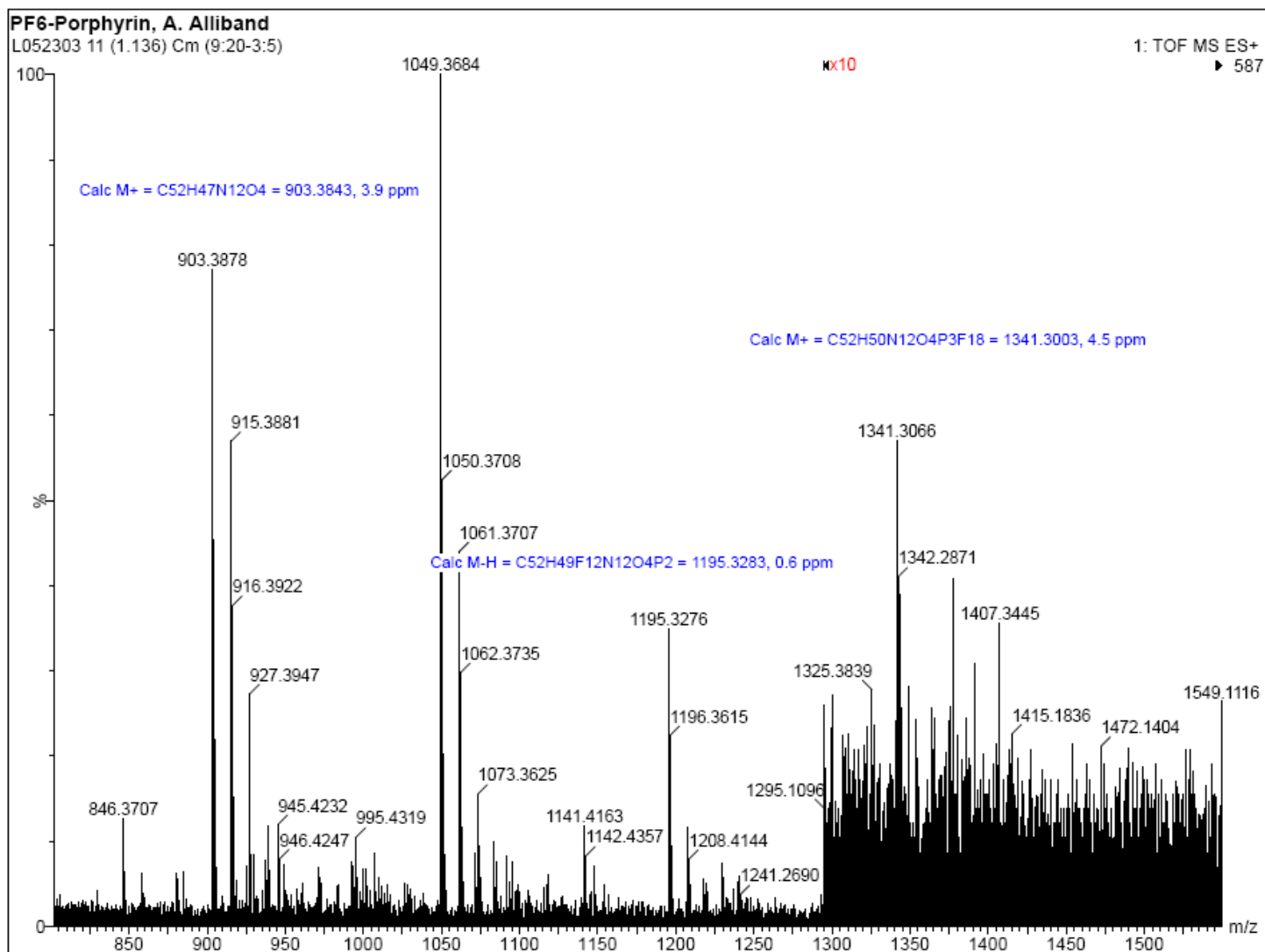
S-Figure 10: ^{19}F NMR of **4b** in DMSO- d_6 (reference is TFA in DMSO- d_6 at -76.55 ppm).



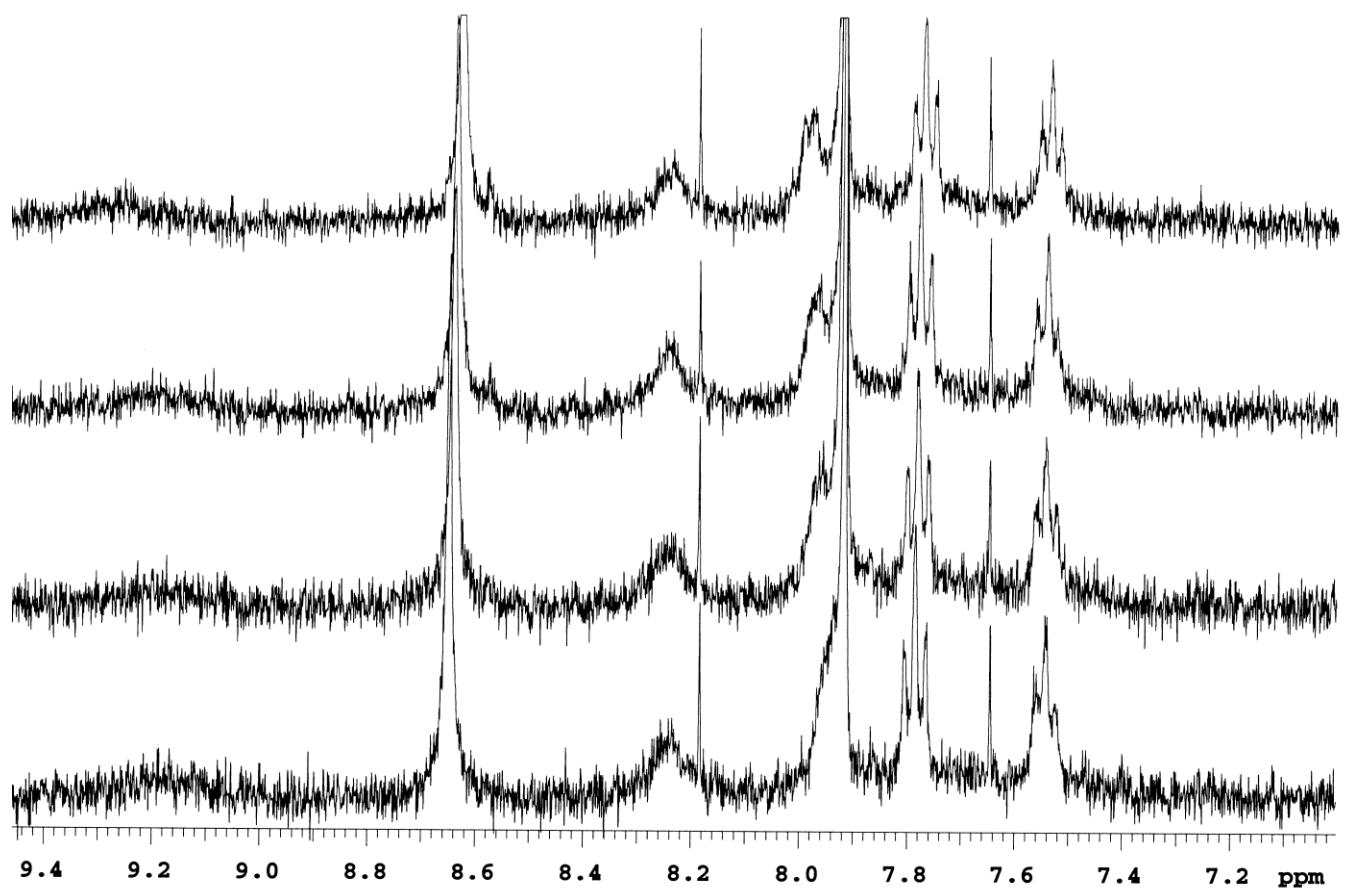
S-Figure 11: ^{31}P NMR of **4b** in DMSO- d_6 (reference is H_2PO_4 in DMSO- d_6 at 0.00 ppm).



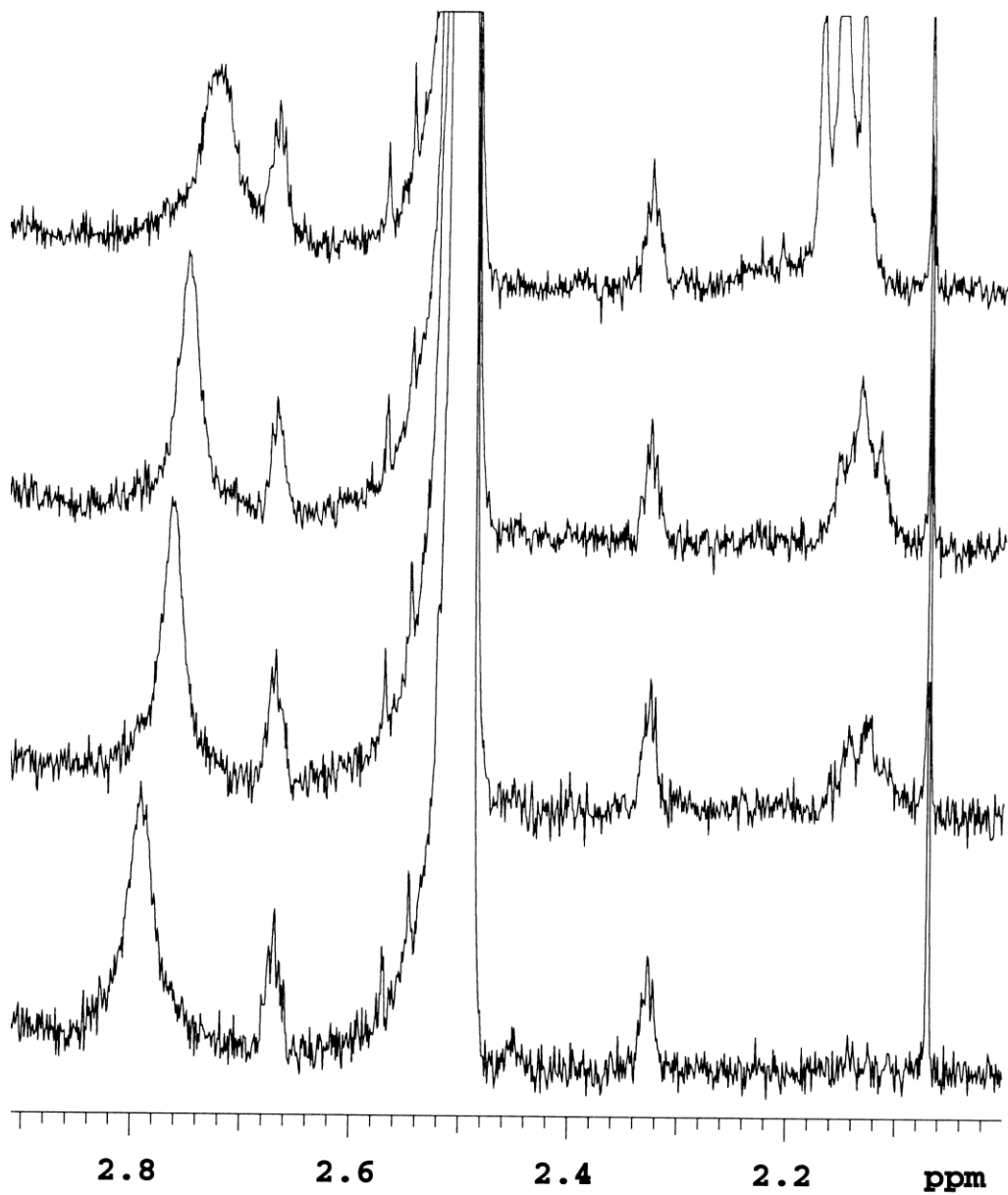
S-Figure 12: ^{31}P NMR of NH_4PF_6 in DMSO- d_6 for comparison



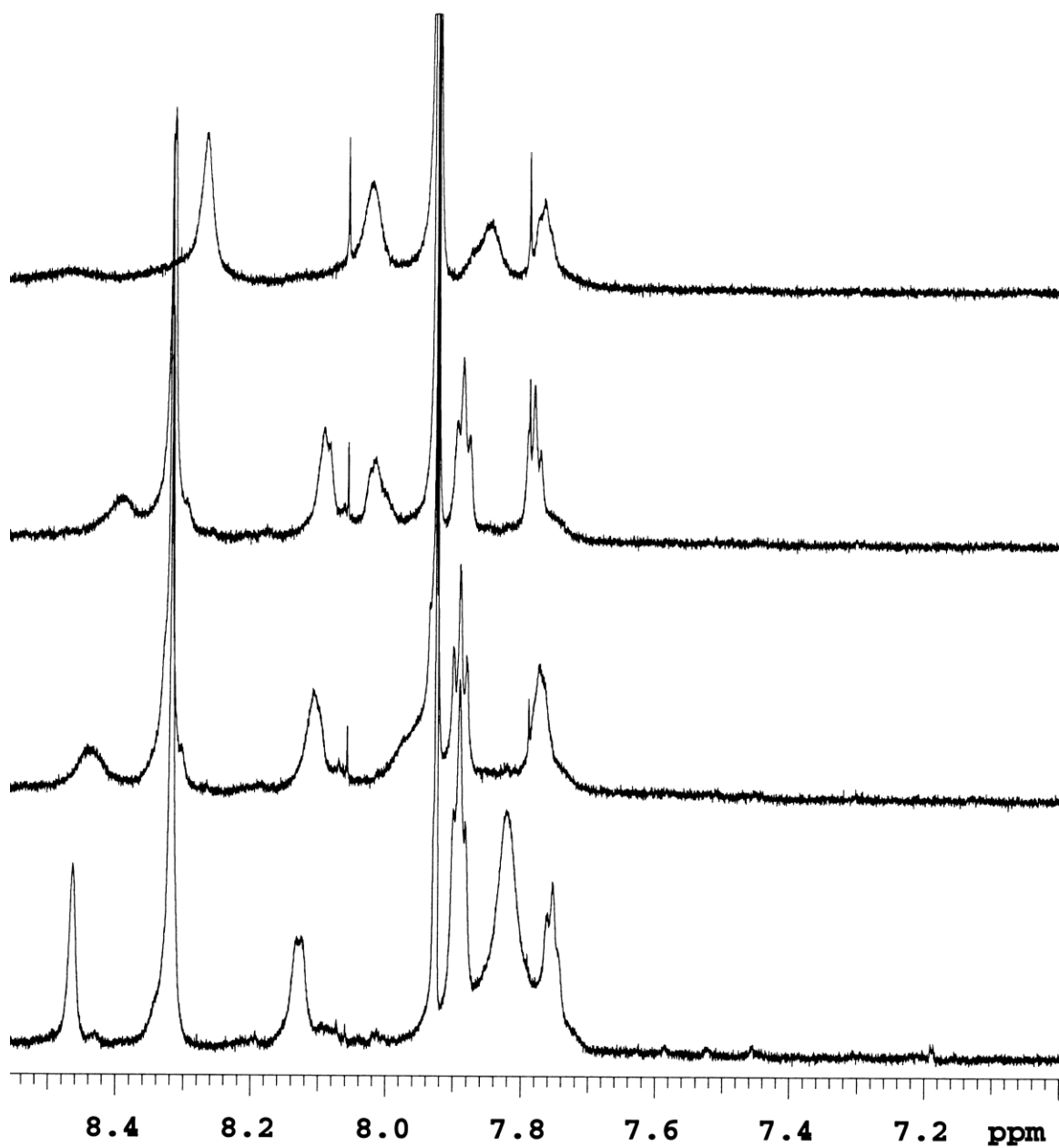
S-Figure 13: HRMS of 4b



S-Figure 14. Stacked plot of partial spectrum from the titration of porphyrin **4b** with TBAPG (60% CDCl₃/40% DMSO-d₆). Equivalents of TBAPG (from bottom to top): 0.0; 0.6; 1.0; 2.5. The broad singlet of the amide protons at 9.18 ppm moves downfield with increased TBAPG equivalents; the ammonium protons at 7.92 ppm also move downfield with increased TBAPG equivalents.

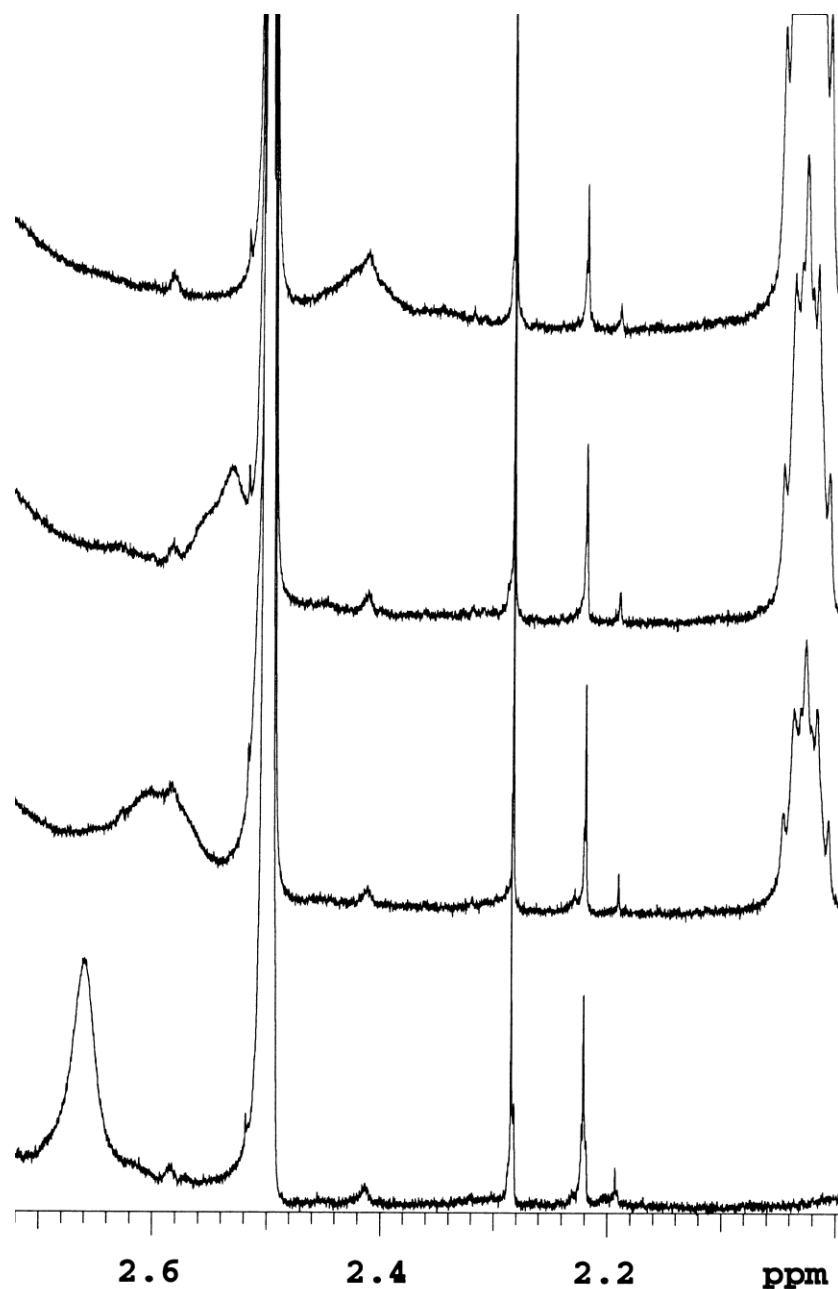


S-Figure 15. Stacked plot of partial spectrum from the titration of **4b** with TBAPG (60% CDCl₃/ 40% DMSO-d₆). Equivalents of TBAPG (from bottom to top): 0.0; 0.6; 1.0; 2.5. The broad singlet of the glycine methylenes at 2.79 ppm moves upfield with increased TBAPG equivalents.

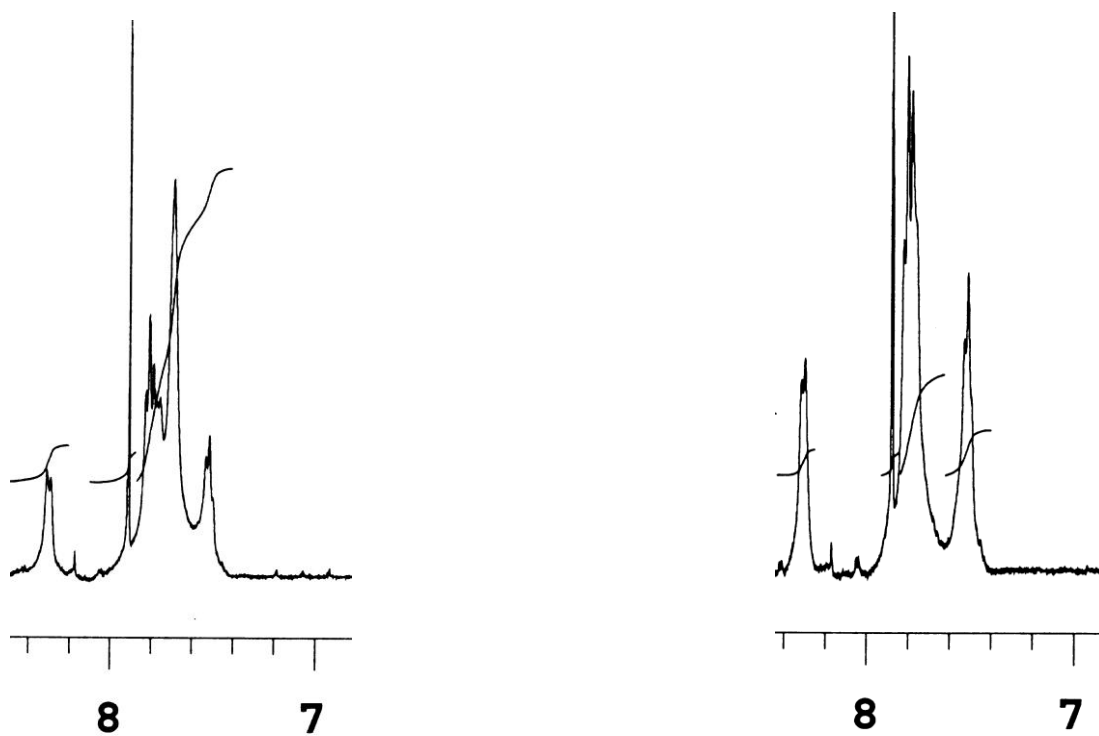


S-Figure 16. Stacked plot of partial spectrum of the titration of **4b** with TBAH₂PO₄ (60% CDCl₃/ 40% DMSO-d₆). Equivalents of TBAH₂PO₄ (from bottom to top) 0.0; 0.6; 1.0; 2.5. Broad singlet of the ammonium protons

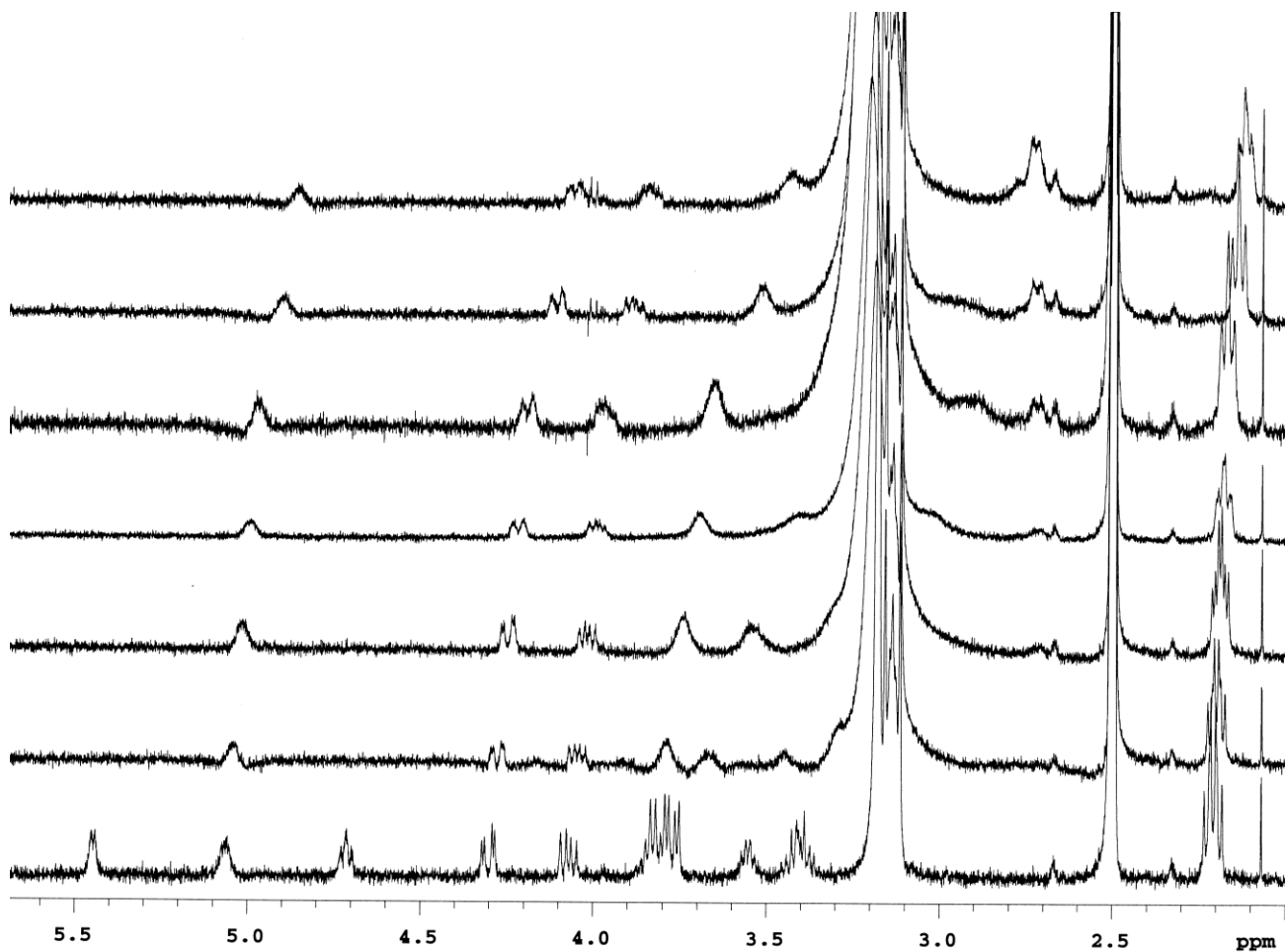
at 7.82 ppm move downfield with increased TBAH_2PO_4 equivalents. Singlet of the amide protons at 8.46 ppm move upfield with increased TBAH_2PO_4 equivalents (up to addition of one equivalent).



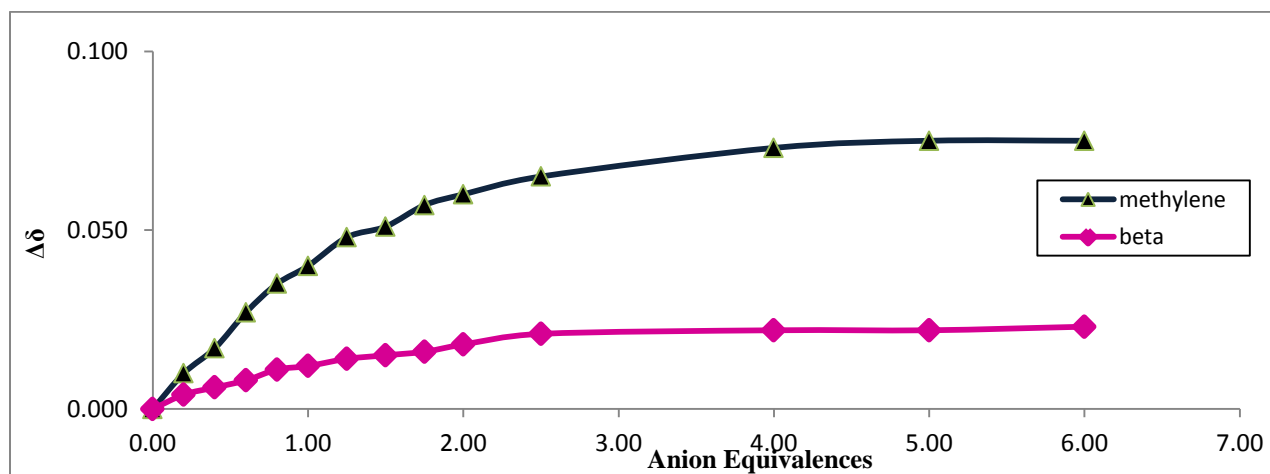
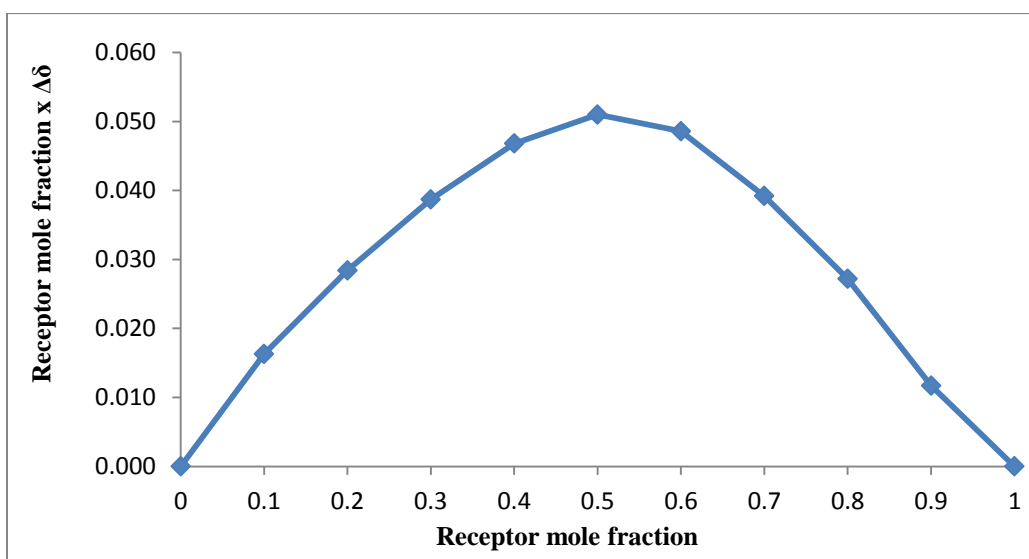
S-Figure 17. Stacked plot of partial spectrum of the titration of **4b** with TBAH_2PO_4 (60% CDCl_3 / 40% DMSO-d_6). Equivalents of TBAH_2PO_4 (from bottom to top) 0.0; 0.6; 1.0; 2.5. Broad singlet of the glycine methylenes at 2.67 ppm move upfield with increased TBAH_2PO_4 equivalents.



S-Figure 18. Partial spectra of **4b** (60% CDCl₃/ 40% DMSO-d₆): Left, proton resonance at 7.7 ppm are the 12 ammonium protons; Right, spectrum after addition of CD₃OD showing deuterium exchange and resultant loss of proton resonance at 7.7 ppm.

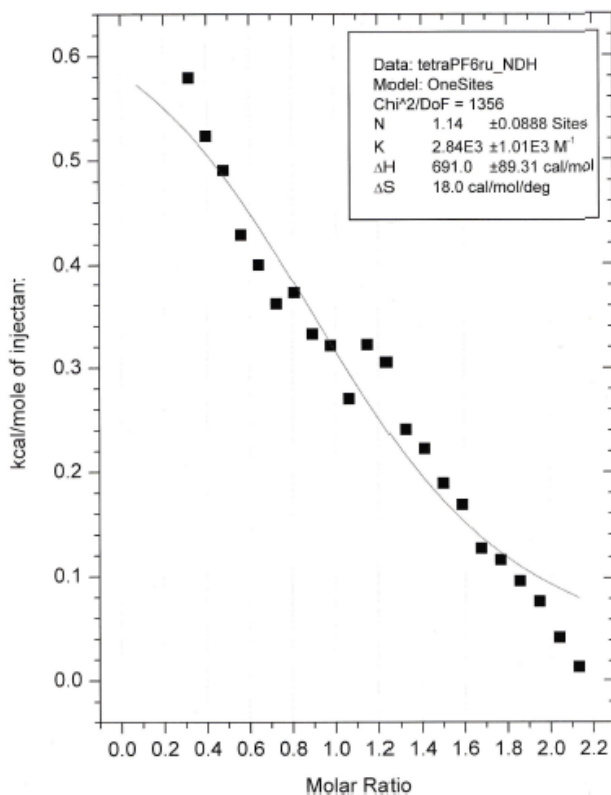
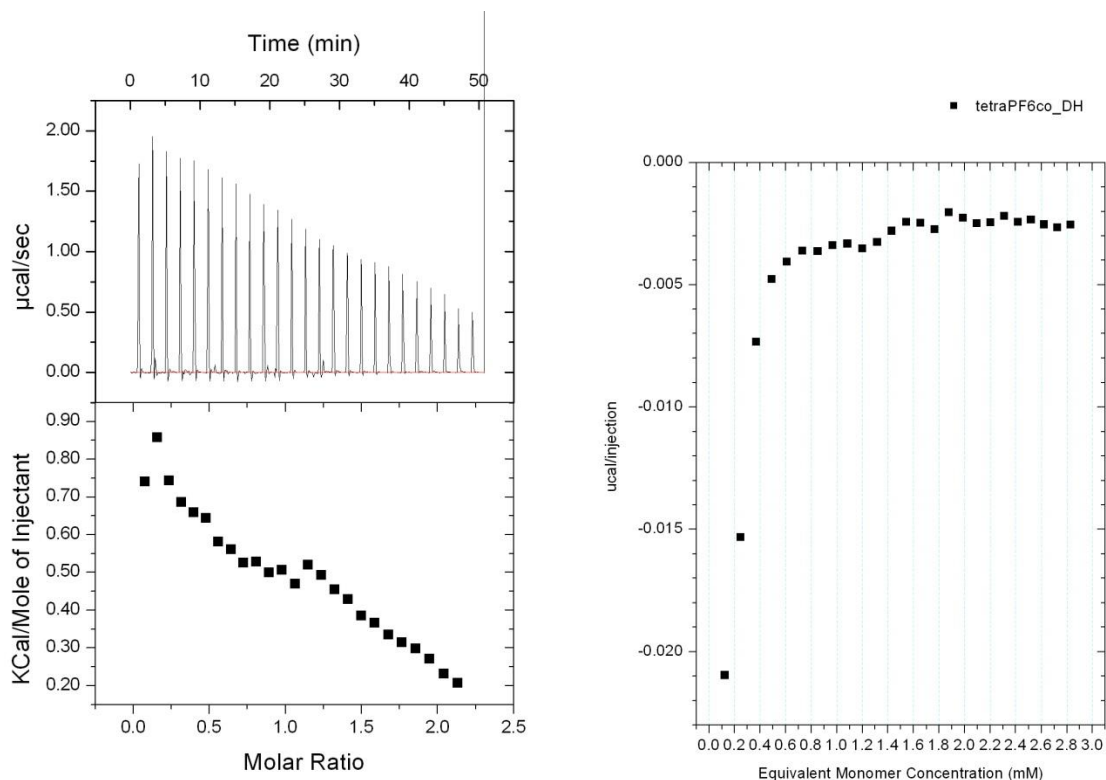


S-Figure 19. Stacked plot partial spectra of the inverse titration of TBAPG (60% CDCl₃/40% DMSO-d₆) with **4b**. Equivalents of **4b** are (from bottom to top): 0.0; 0.05; 0.10; 0.15; 0.20; 0.4; 0.6. Multiplets in the region between 3.35-3.85 ppm that correspond to the lipid's glycerol headgroup protons move quickly upfield with increasing equivalents of **4b**.

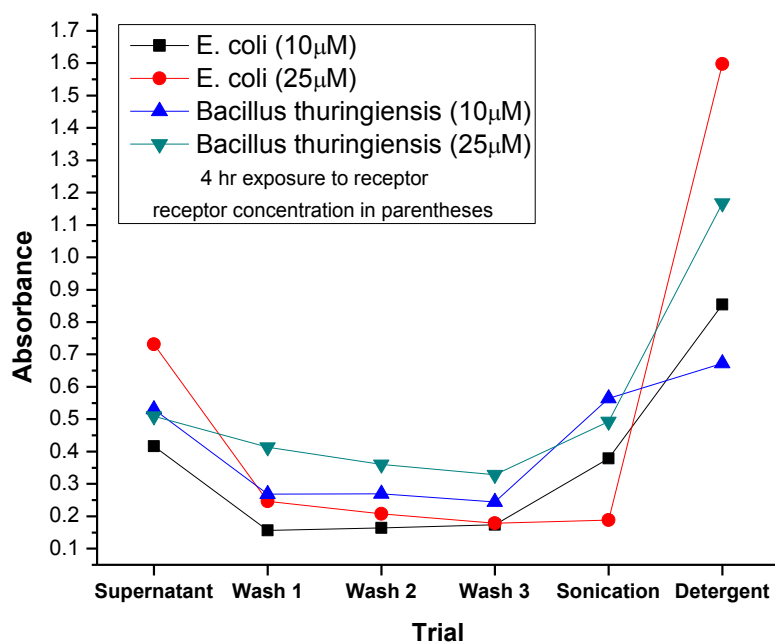
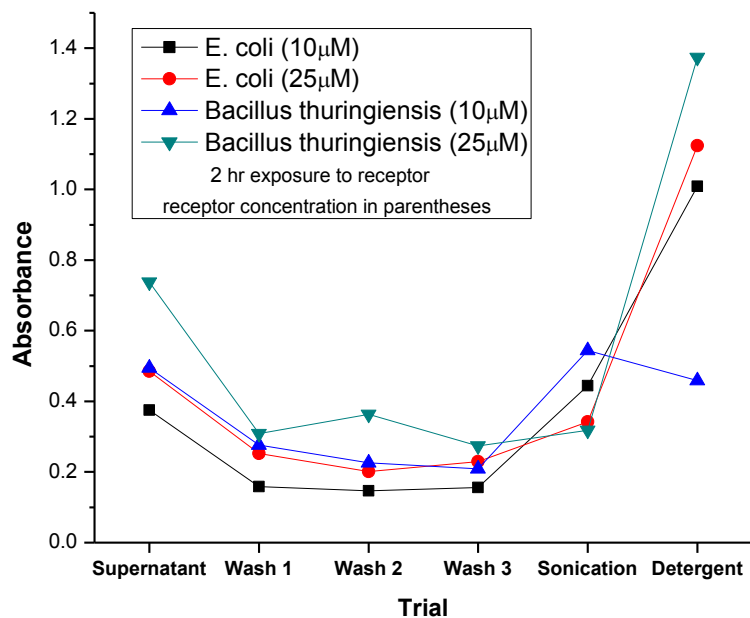


S-Figure 20: Representative example of ^1H NMR titration experiments in 40% DMSO/ 60% CHCl_3 at 30 $^\circ\text{C}$.

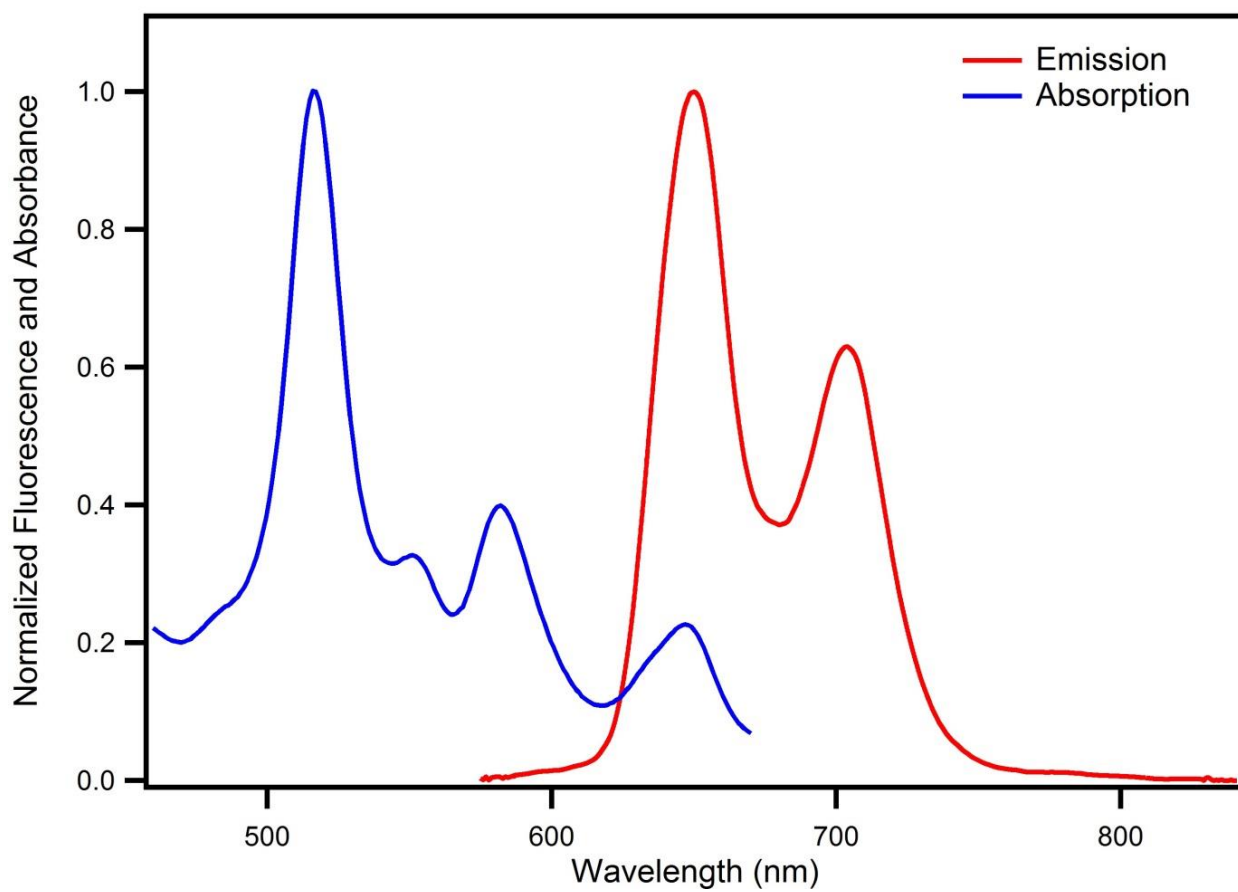
Upper: Job plot for TBAPG and **4b** (**4b** mole fraction plotted on x-axis); Bottom: Binding isotherms for the titration of **4b** with TBAPG. The JOB experiments and titration experiments were conducted at slightly different concentrations to remove any artifacts caused by different concentrations when using ^1H NMR.



S-Figure 21: Representative example of ITC experiment in 50% DMSO/ 45% CHCl₃/ 5% CH₃OH at 40 °C. Upper left: ITC data for the TBAPG addition to **4b**; Upper right: ITC data for the control addition of TBAPG to solvent system; Bottom: Corrected ITC curve for the addition of TBAPG to **4b** after subtraction of control curve.



S-Figure 22: Absorbance (420 nm) of supernatants of various trials with *E. coli* and *Bacillus thuringiensis* after incubation of the receptor **4a** (10 or 25 μM) with the bacterial solutions for: Top 2 hr; Bottom 4 hr.



S-Figure 23: Normalized absorption spectrum and emission spectrum (excited at 514 nm) of receptor **4a** in HEPES buffer solution (25 mM) containing Na₂SO₄ (50 mM) at pH 6.5.

