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

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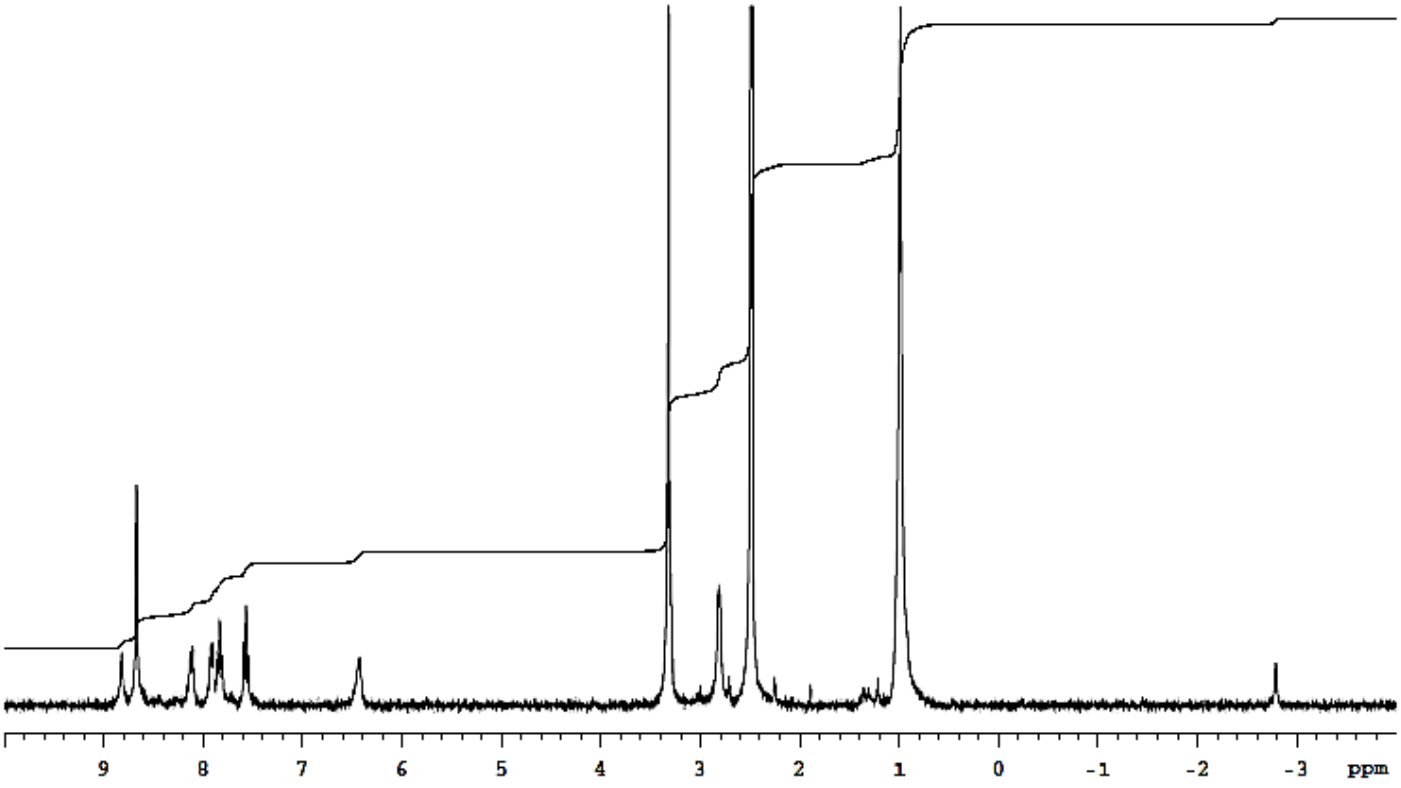
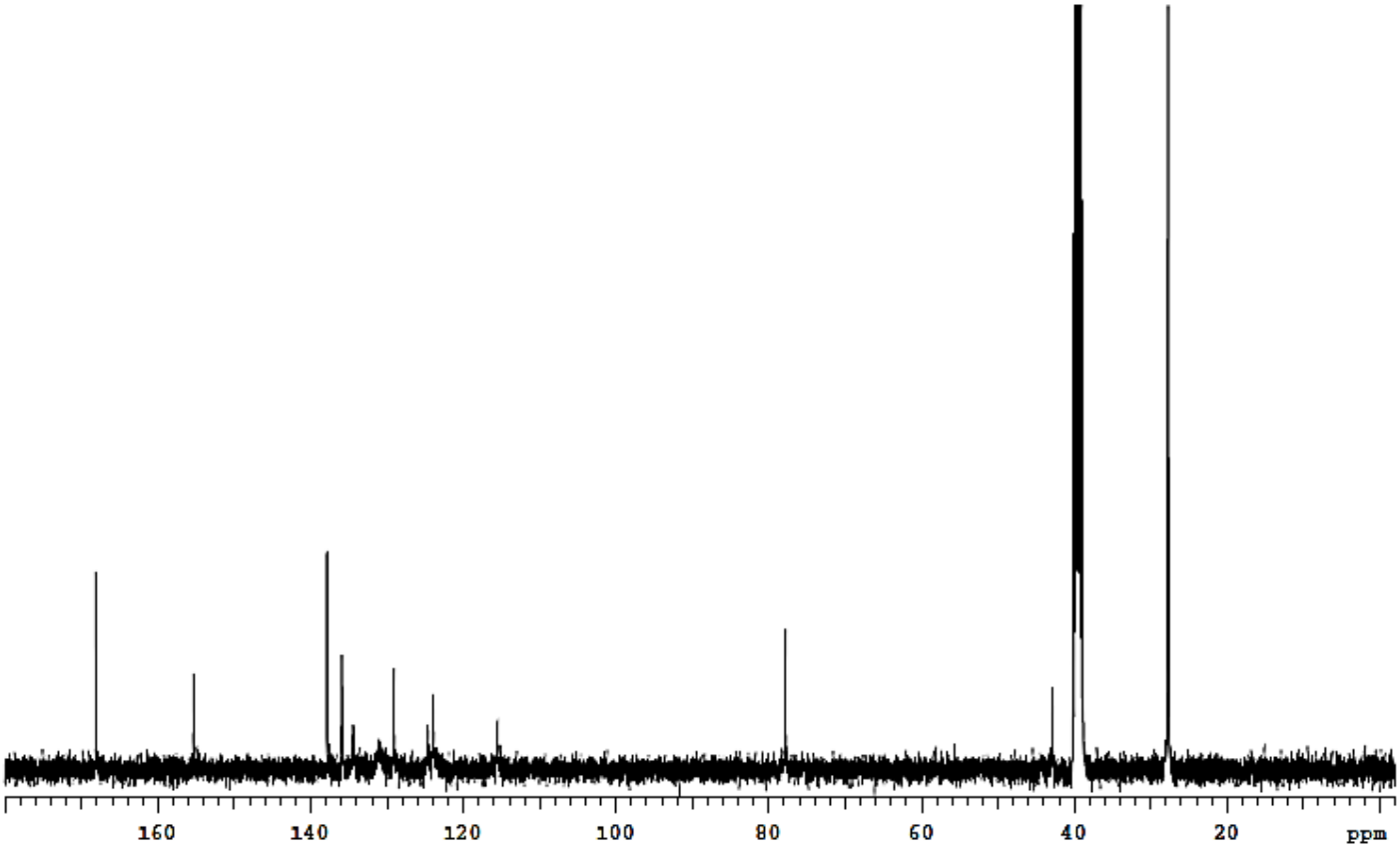
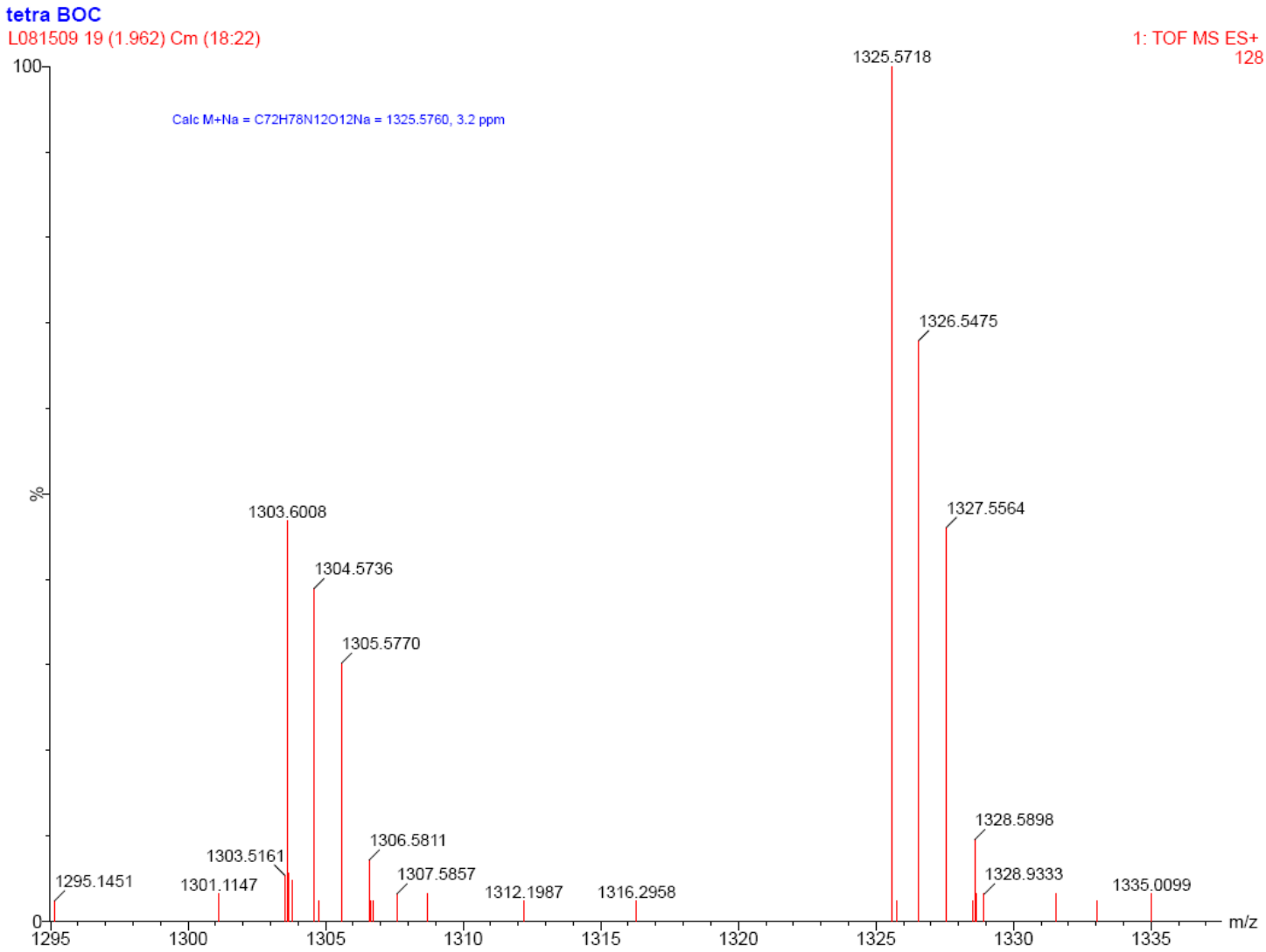


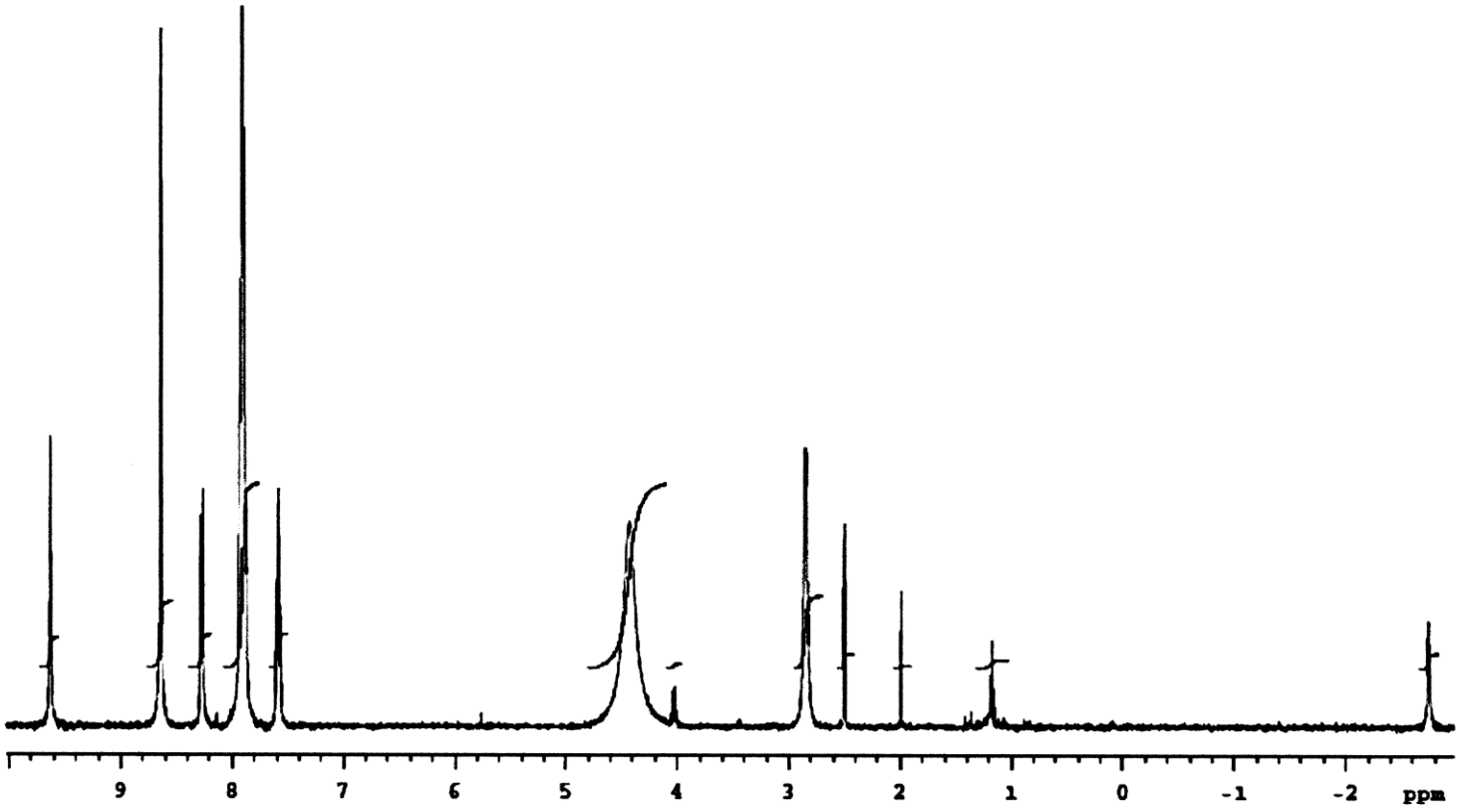
S-Figure 1: ^{1}H NMR of **3** in DMSO-d_6



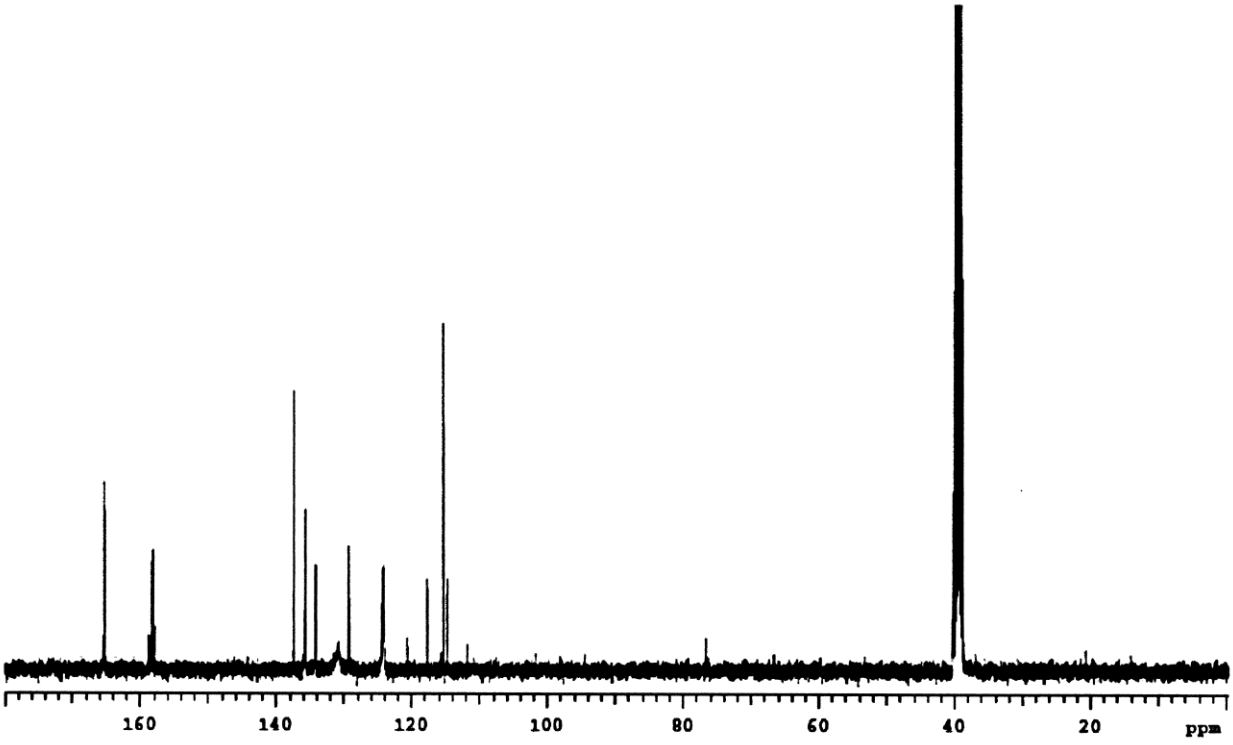
S-Figure 2: ^{13}C NMR of **3** in DMSO-d_6



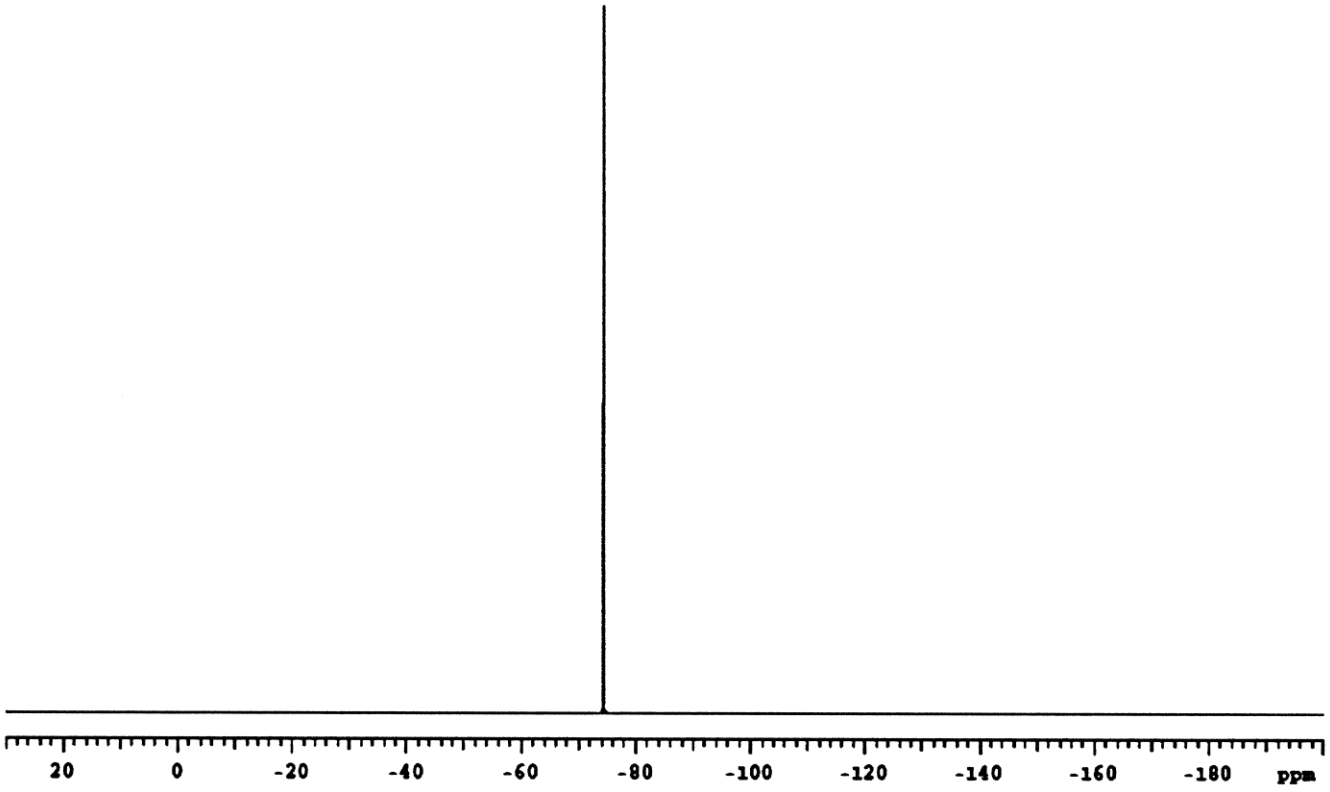
S-Figure 3: HRMS of **3**



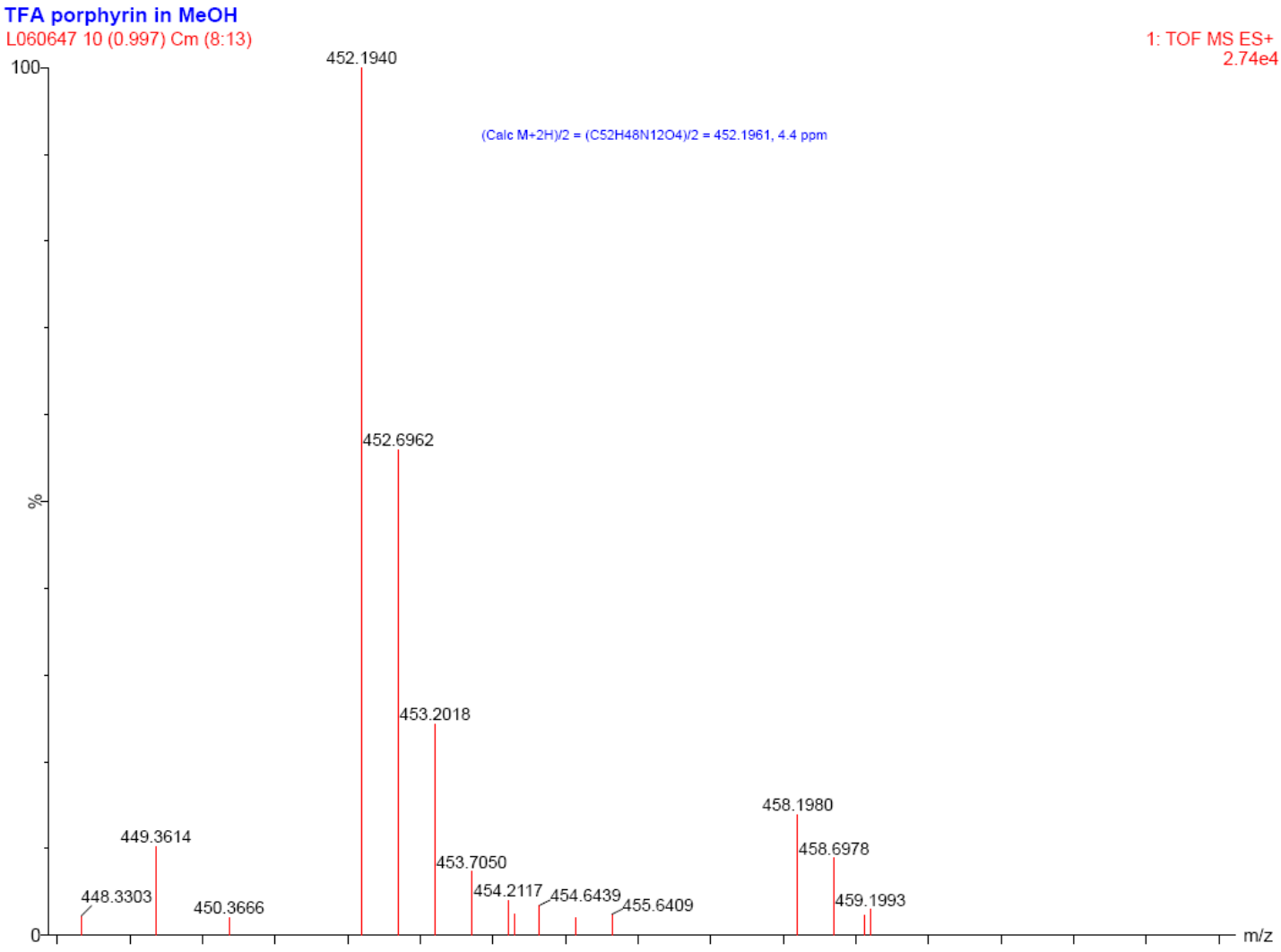
S-Figure 4: ^{1}H NMR of **4a** in DMSO-d_6 (resonances at 4.0, 2.0, and1.15 ppm are ethyl acetate solvent)



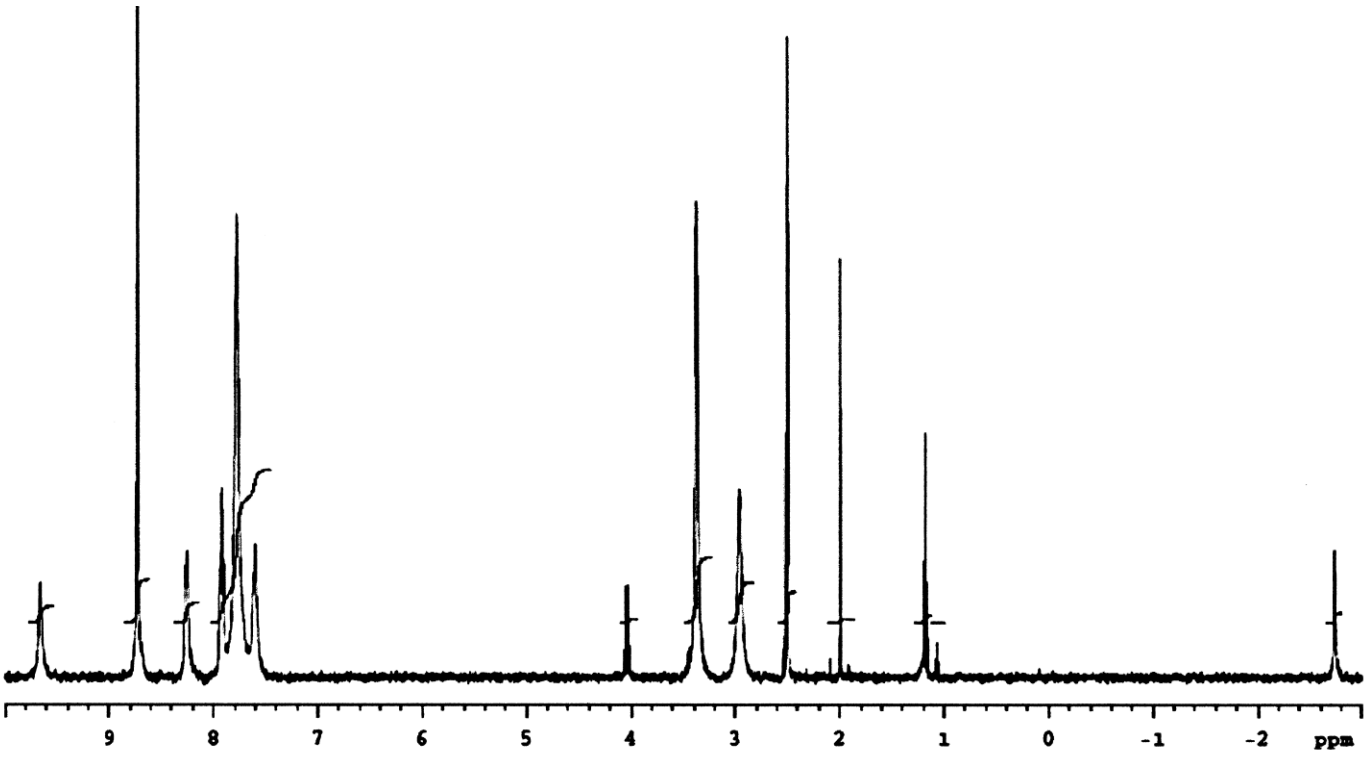
S-Figure 5: ^{13}C NMR of **4a** in DMSO-d_6



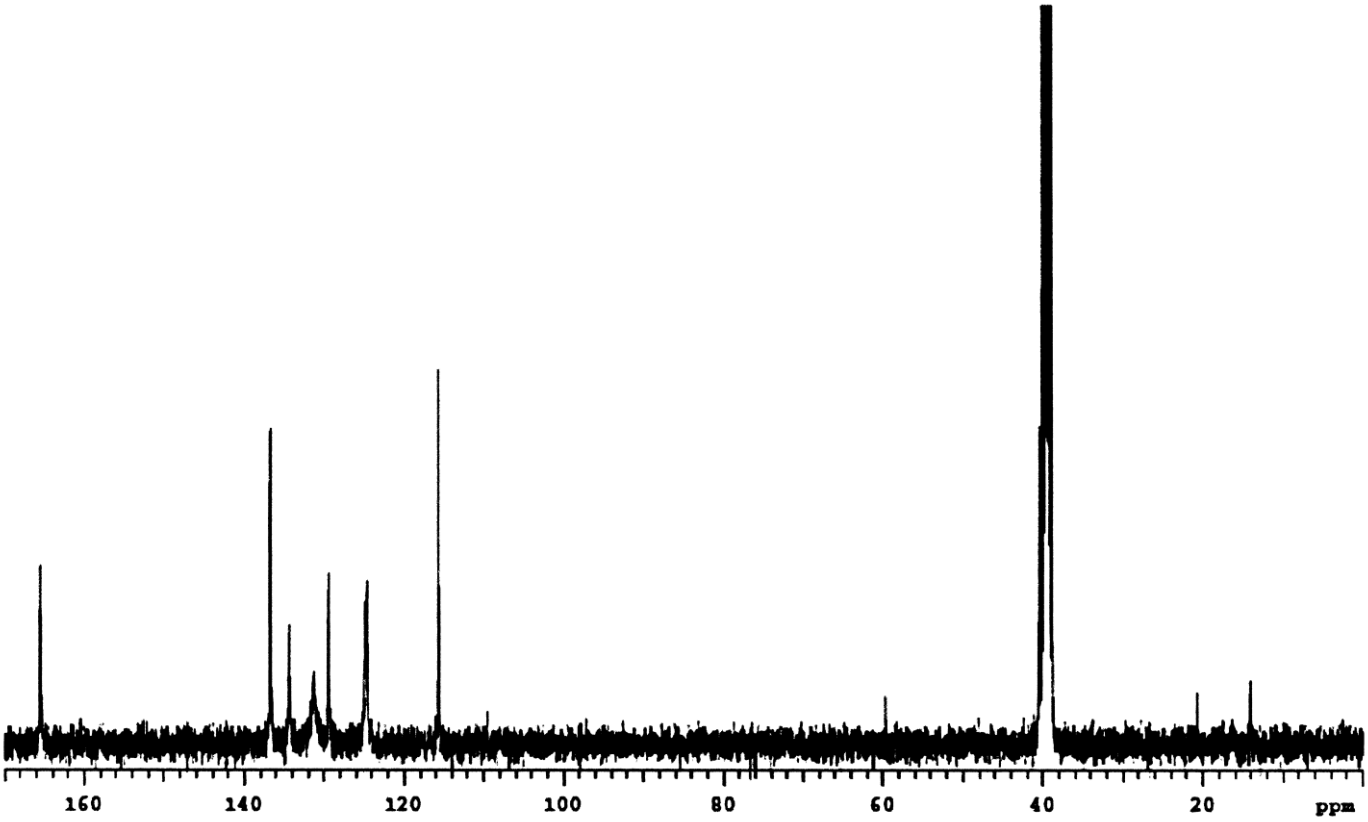
S-Figure 6: ^{19}F NMR of **4a** in DMSO-d_6 (reference is TFA in DMSO-d_6 at -76.55 ppm).



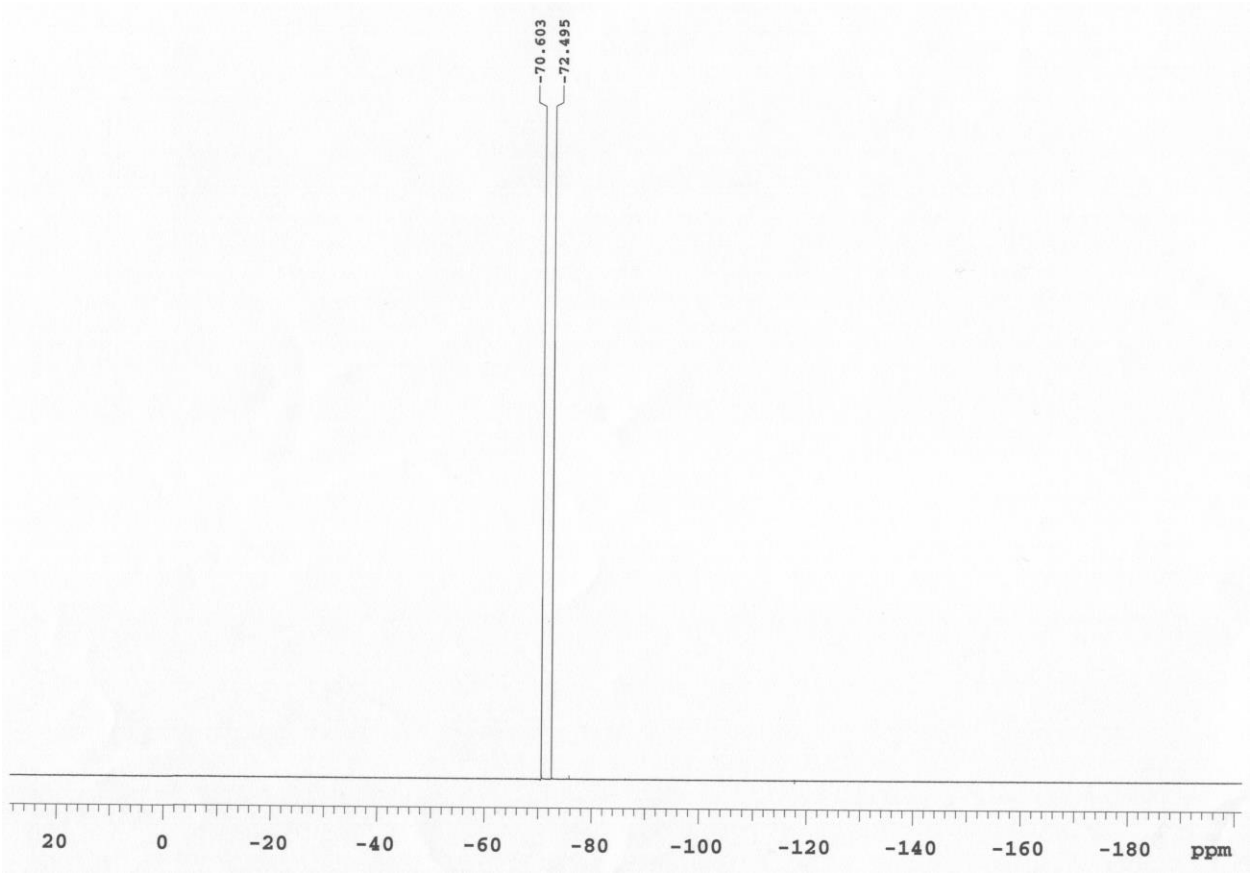
S-Figure 7: ESI HRMS of **4a**.



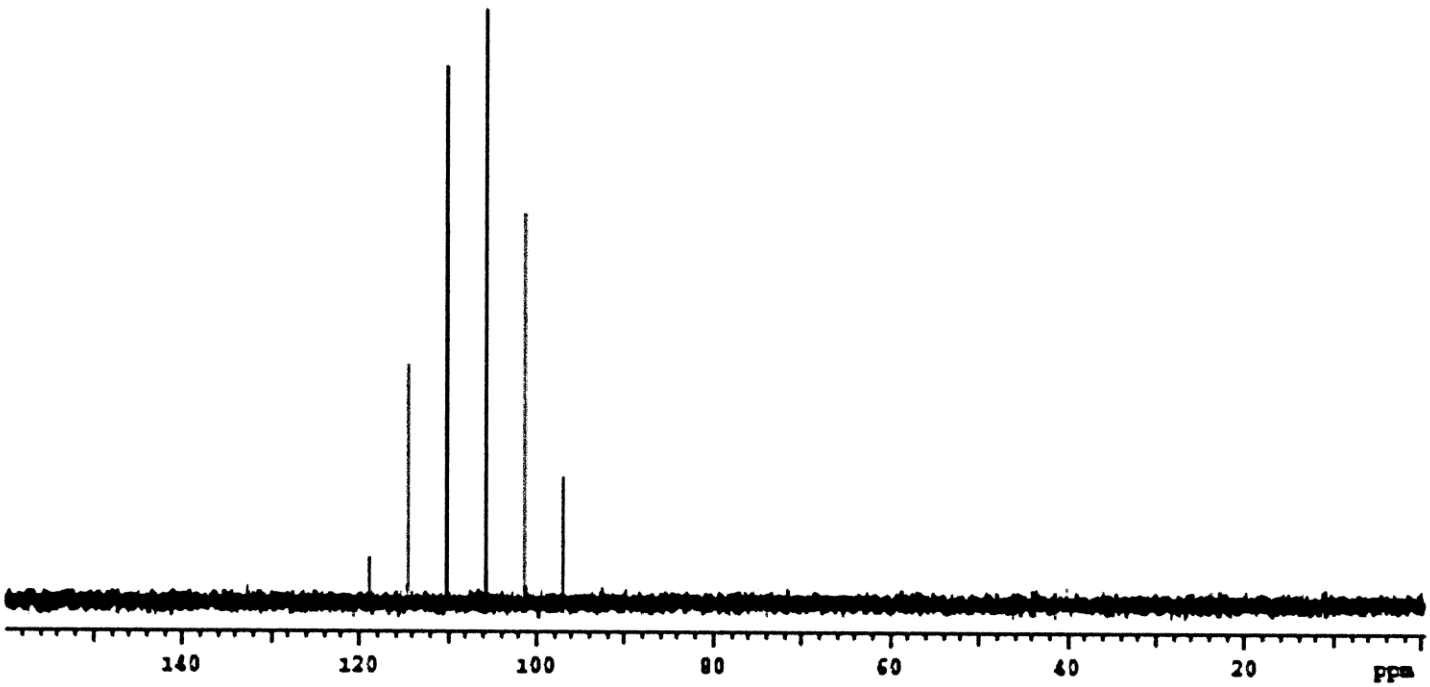
S-Figure 8: ^{1}H NMR of **4b** in DMSO-d_6 (resonances at 4.0, 2.0, and1.15 ppm are ethyl acetate solvent)



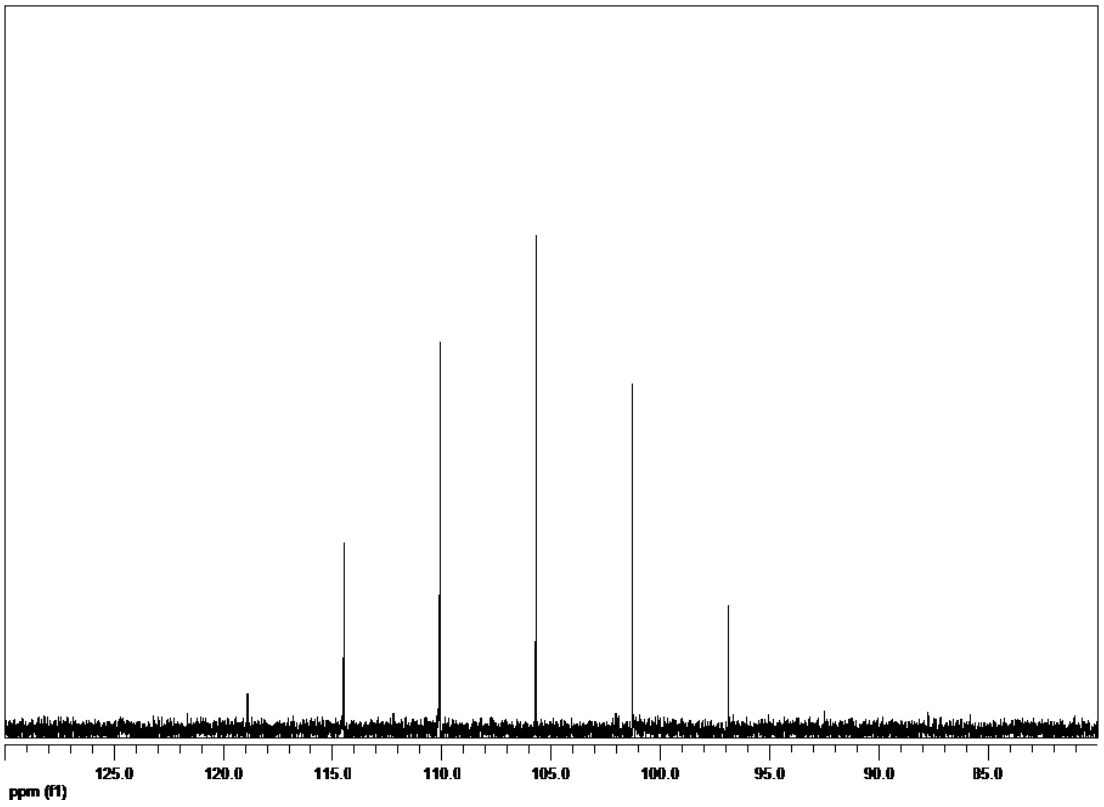
S-Figure 9: ^{13}C NMR of **4b** in DMSO-d_6



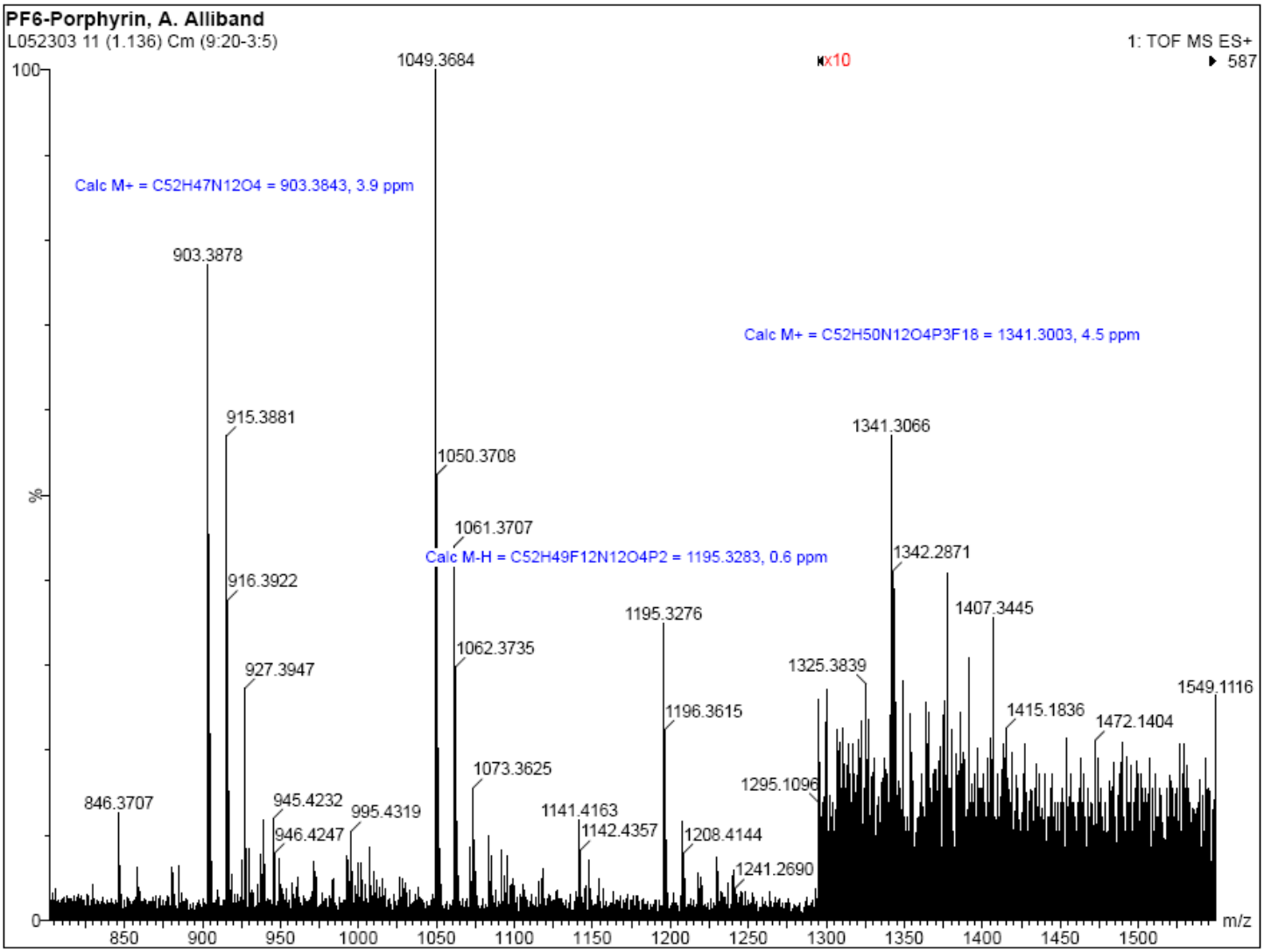
S-Figure 10: ^{19}F NMR of **4b** in DMSO-d_6 (reference is TFA in DMSO-d_6 at -76.55 ppm).



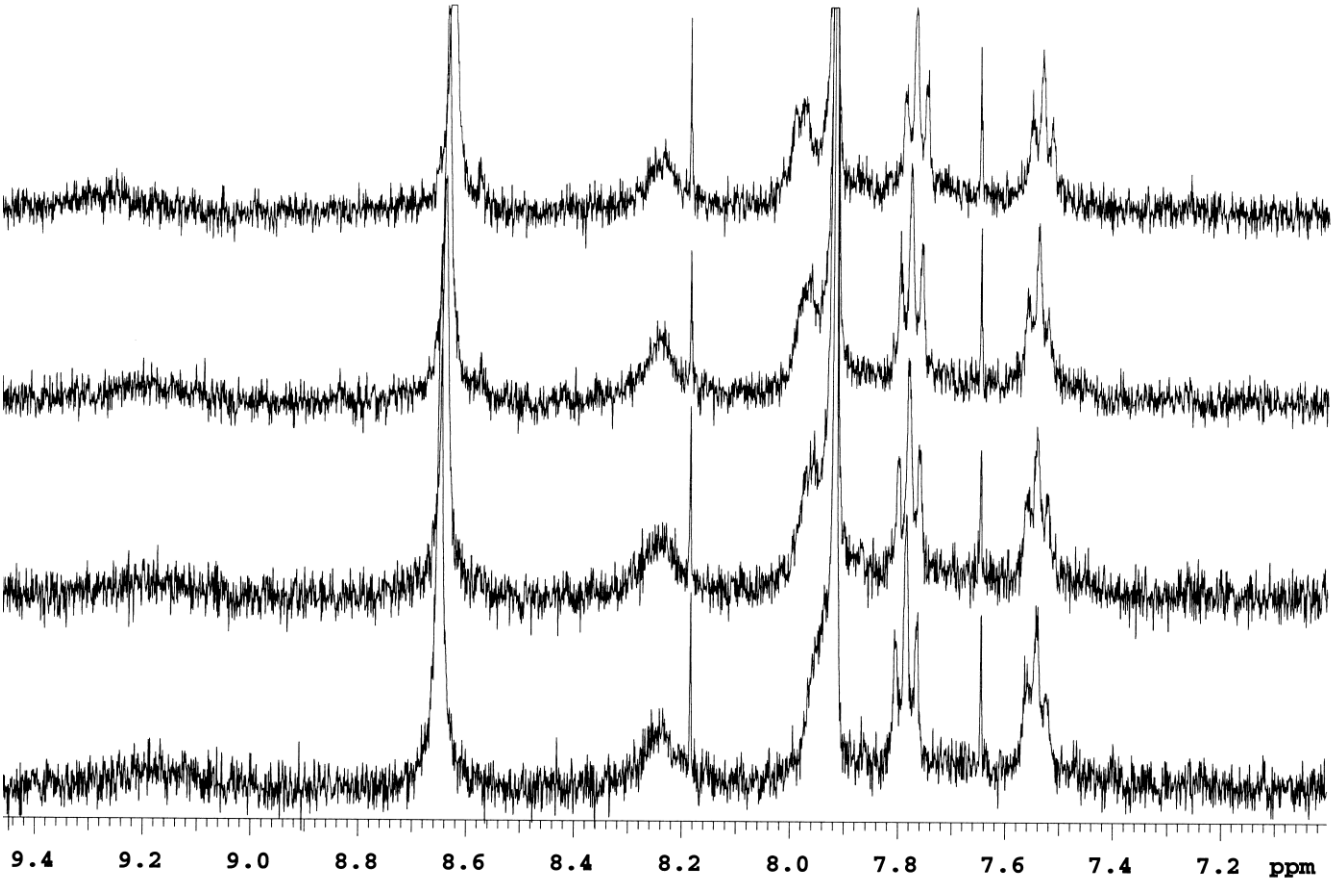
S-Figure 11: ^{31}P NMR of **4b** in DMSO-d_6 (reference is H_2PO_4 in DMSO-d_6 at 0.00 ppm).



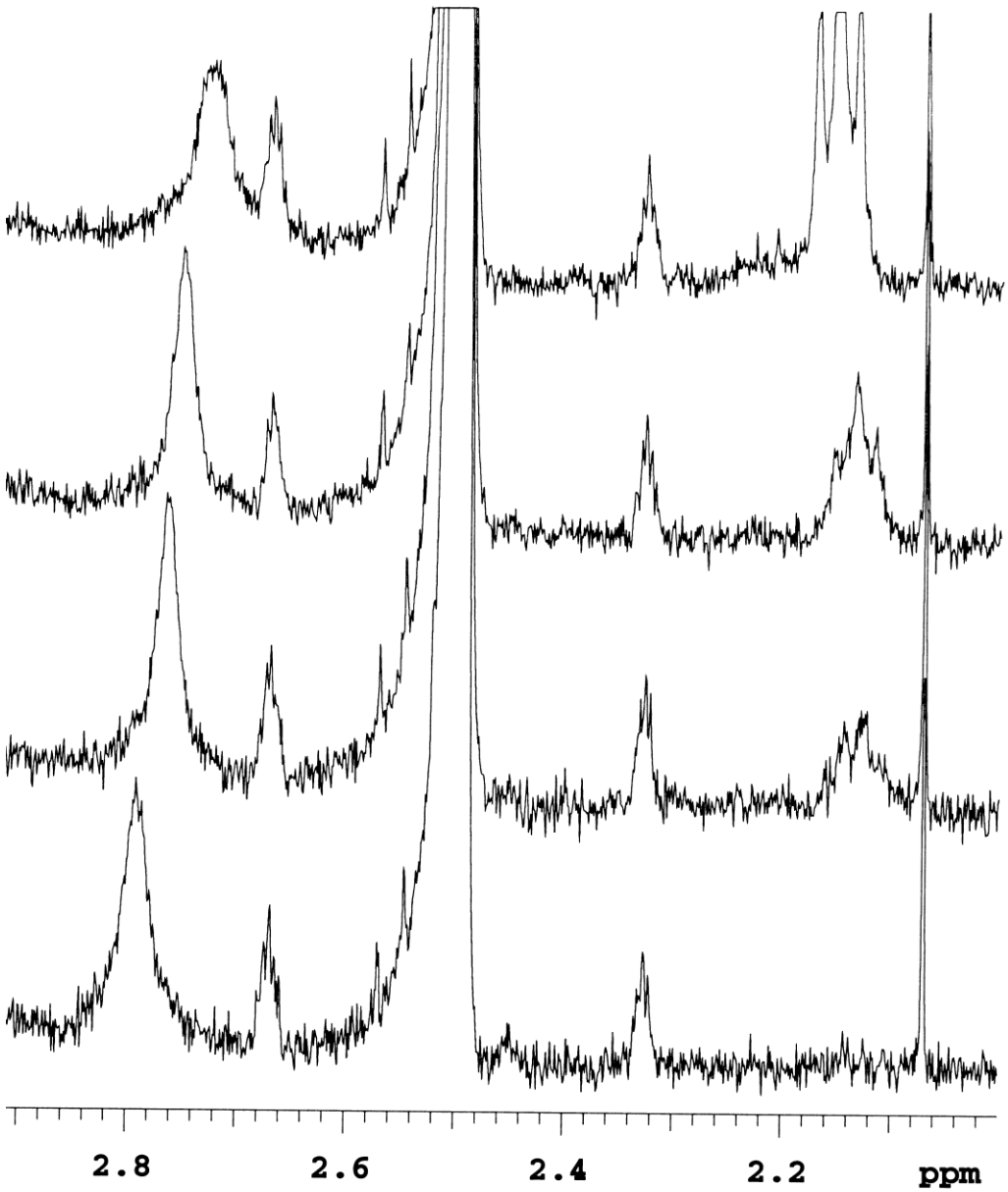
S-Figure 12: ^{31}P NMR of NH_4PF_6 in DMSO-d_6 for comparison



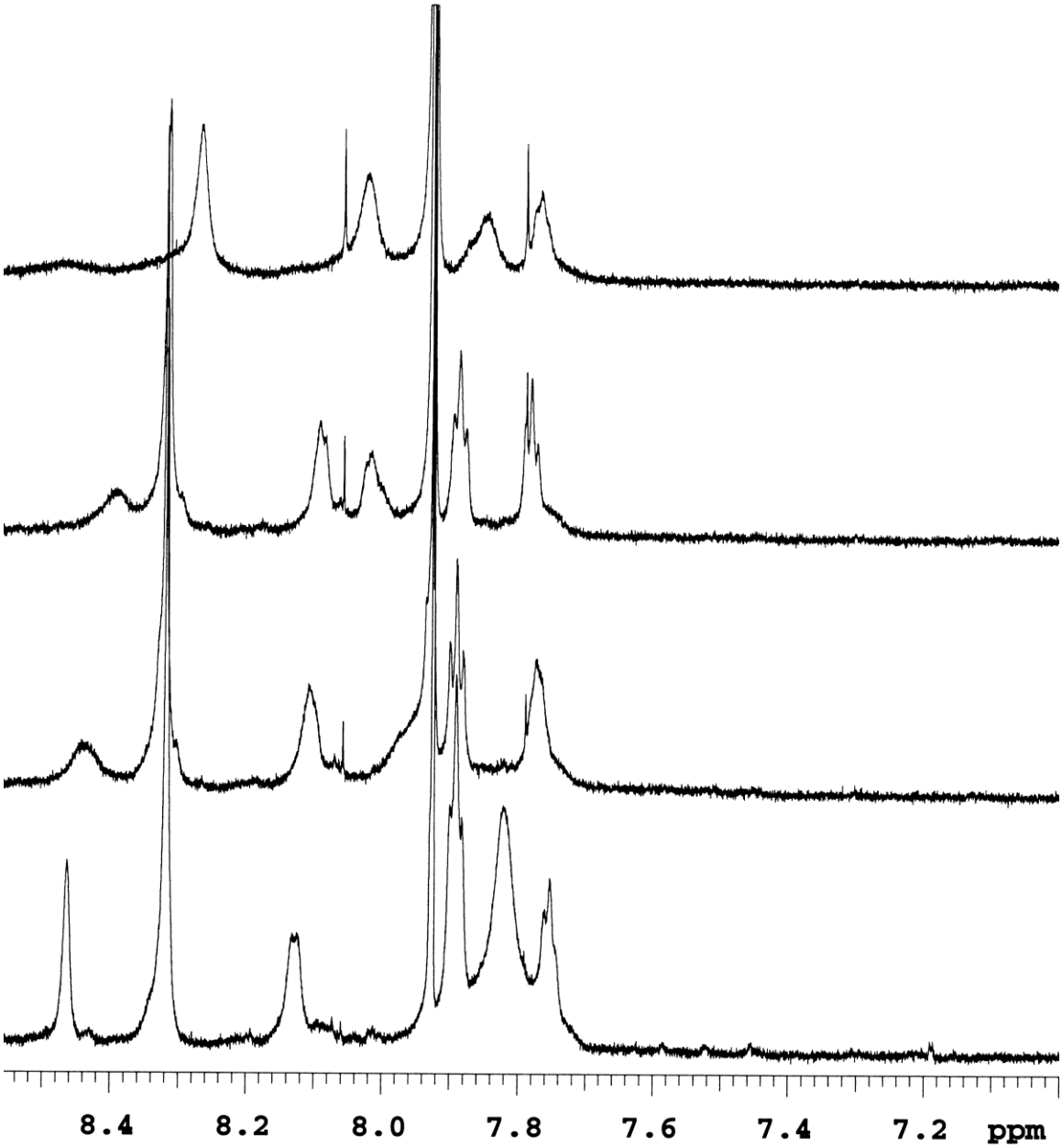
S-Figure 13: HRMS of **4b**



S-Figure 14. Stacked plot of partial spectrum from the titration of porphyrin **4b** with TBAPG (60% $CDCl_3$/ 40% DMSO-d_6). 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.

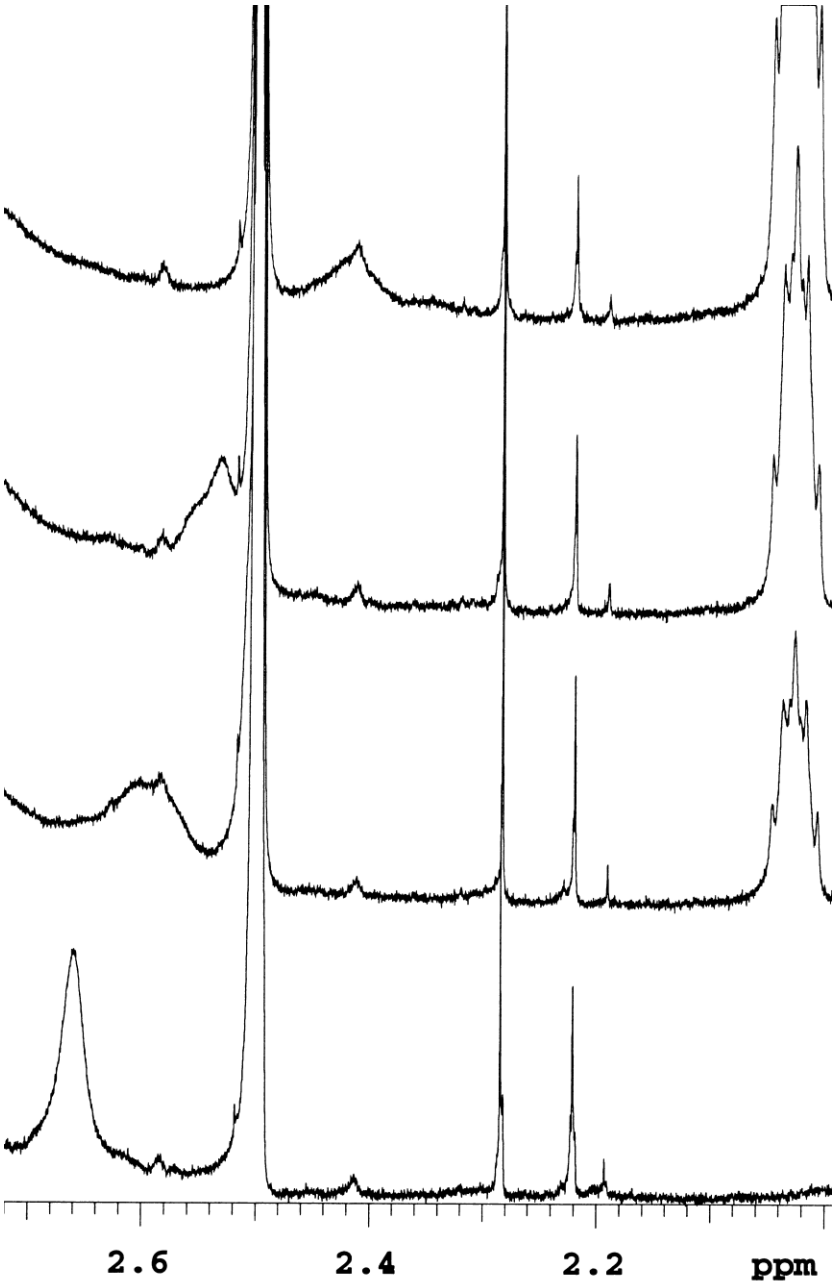


S-Figure 15. Stacked plot of partial spectrum from the titration of **4b** with TBAPG (60% $CDCl_3$/ 40% DMSO-d_6). Equivalents of TBAPG (from bottom to top):0.0; 0.6; 1.0; 2.5. The broad singlet of the glycine methylenes at 2.79 ppm moves upfield with increased TBAPG equivalents.

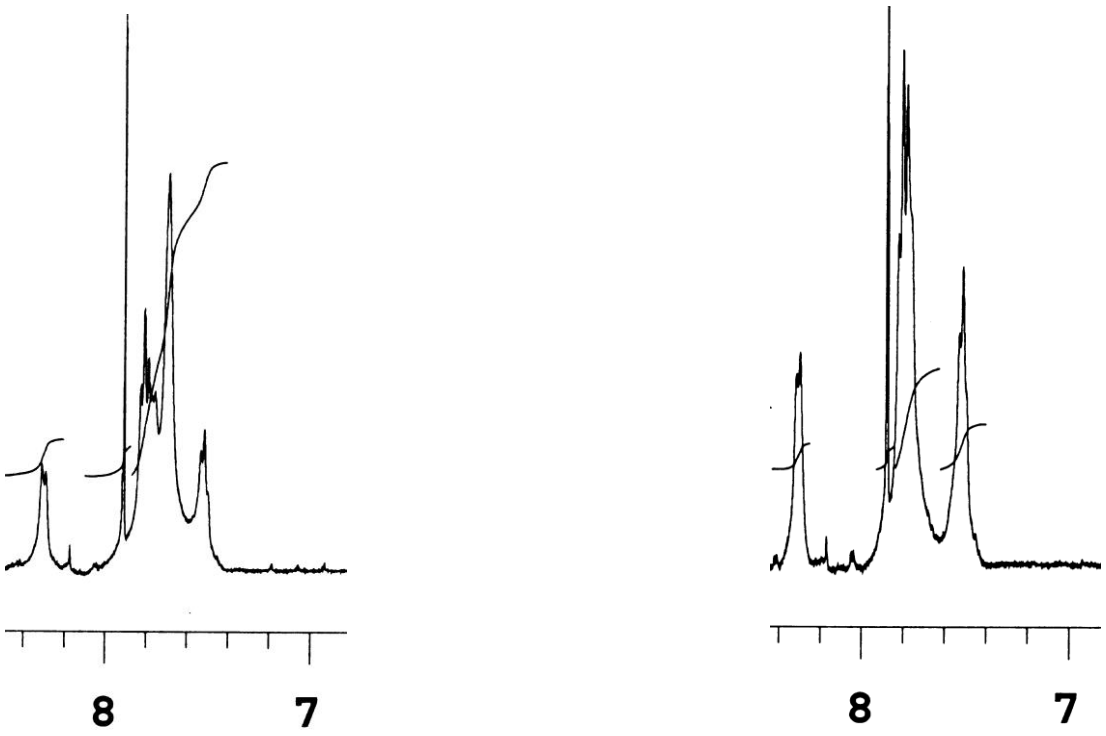


S-Figure 16. Stacked plot of partial spectrum of the titration of **4b** with $TBAH_2PO_4$ (60% $CDCl_3$/ 40% DMSO-d_6). Equivalents of $TBAH_2PO_4$ (from bottom to top) 0.0; 0.6; 1.0; 2.5. Broad singlet of the ammonium protons

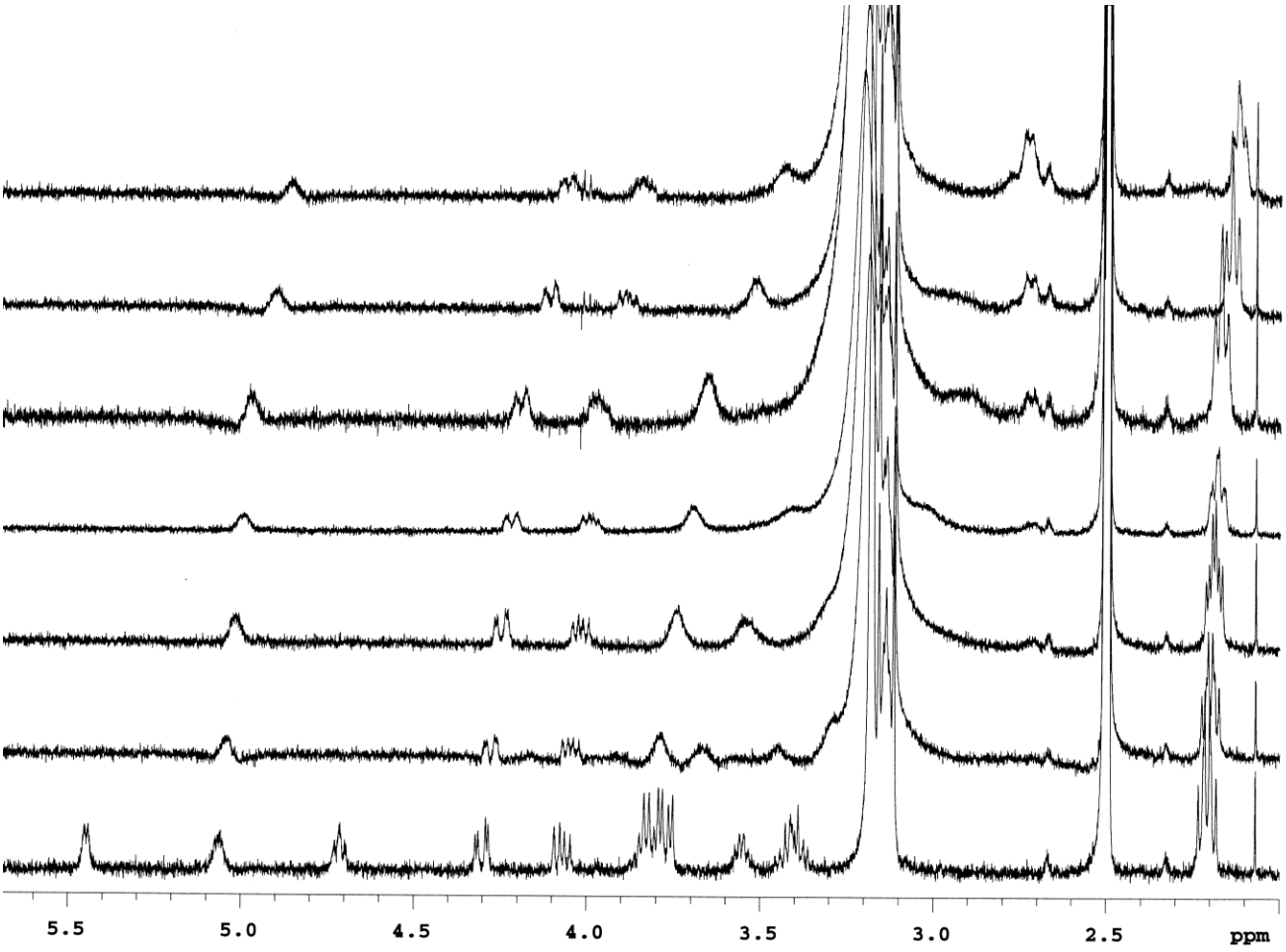
at 7.82 ppm move downfield with increased $TBAH_2PO_4$ equivalents. Singlet of the amide protons at 8.46 ppm move upfield with increased $TBAH_2PO_4$ equivalents (up to addition of one equivalent).



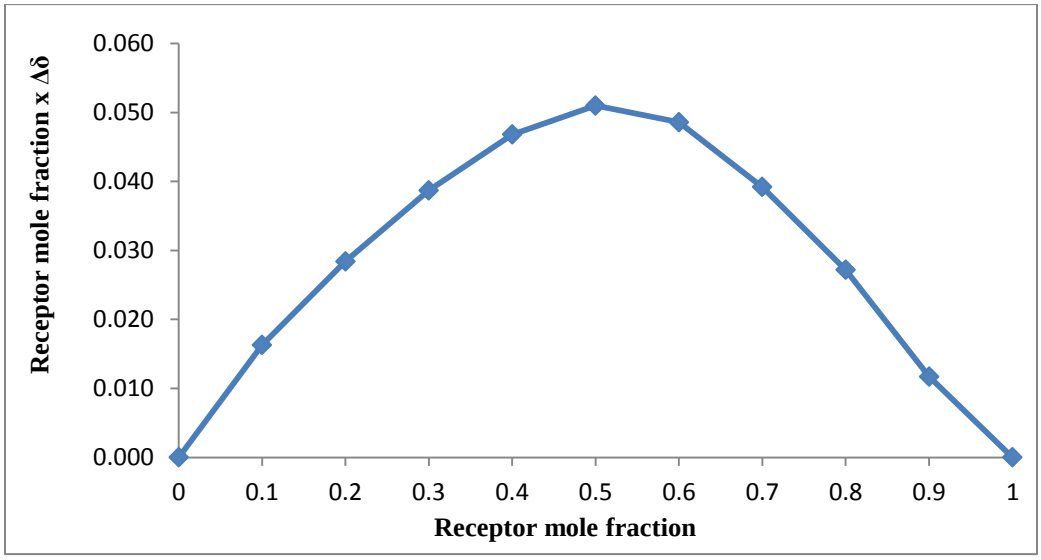
S-Figure 17. Stacked plot of partial spectrum of the titration of **4b** with $TBAH_2PO_4$ (60% $CDCl_3$/ 40% DMSO-d_6). Equivalents of $TBAH_2PO_4$ (from bottom to top) 0.0; 0.6; 1.0; 2.5. Broad singlet of the glycine methylenes at 2.67 ppm move upfield with increased $TBAH_2PO_4$ equivalents.

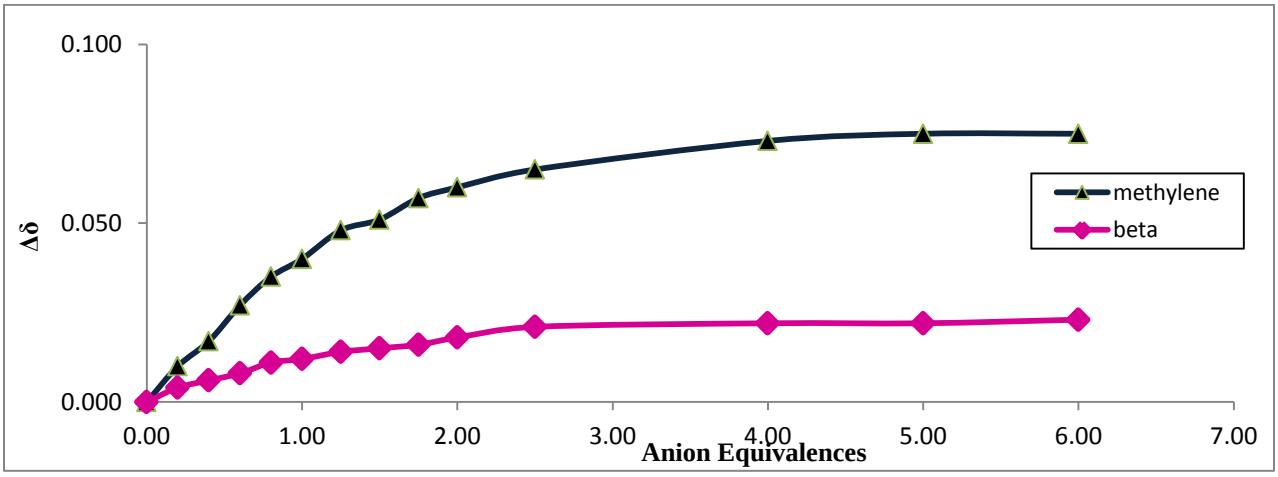


S-Figure 18. Partial spectra of **4b** (60% $CDCl_3$/ 40% DMSO-d_6): Left, proton resonance at 7.7 ppm are the 12 ammonium protons; Right, spectrum after addition of CD_3OD showing deuterium exchange and resultant loss of proton resonance at 7.7 ppm.



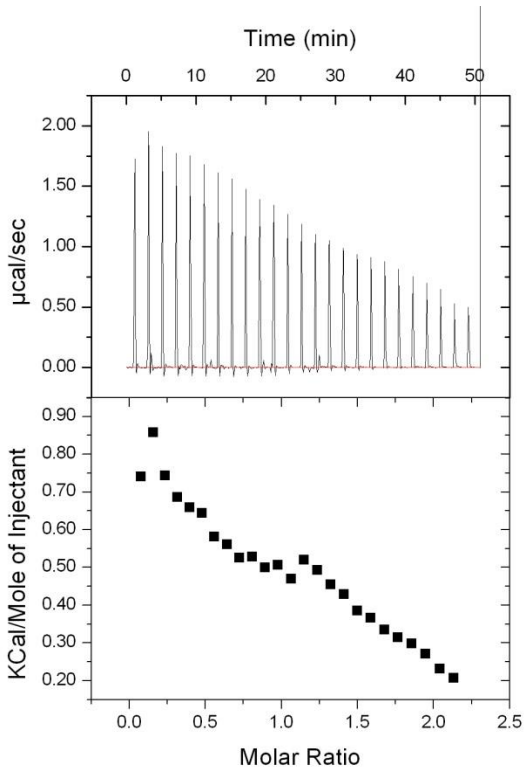
S-Figure 19. Stacked plot partial spectra of the inverse titration of TBAPG (60% $CDCl_3$/40% DMSO-d_6) with **4b**. Equivalents of **4b** are (from bottom to top): 0.0; 0.05; 0.10; 0.15; 0.20; 0.4; 0.6. Multiplets in the region between 3.35-3.85 ppm that correspond to the lipid's glycerol headgroup protons move quickly upfield with increasing equivalents of **4b**.

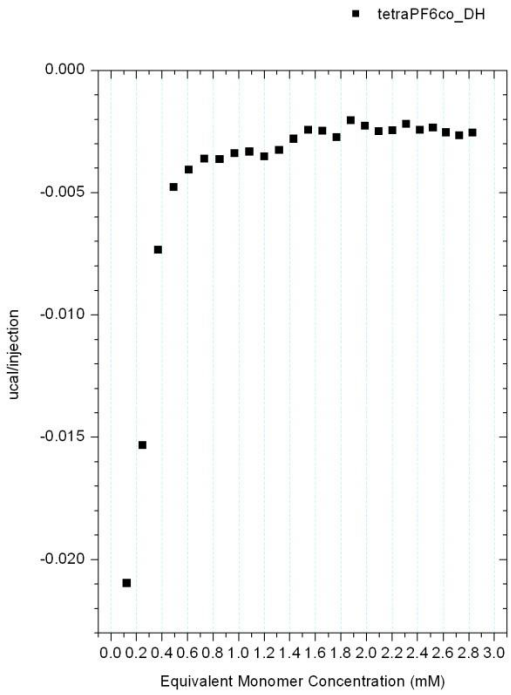


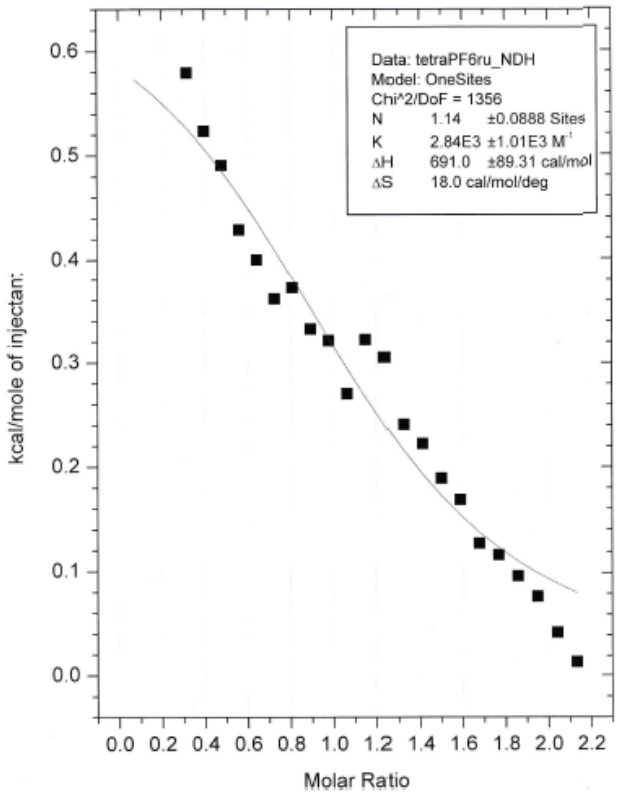


S-Figure 20: Representative example of ^{1}H NMR titration experiments in 40% DMSO/ 60% CHCl3 at 30 ^{o}C.

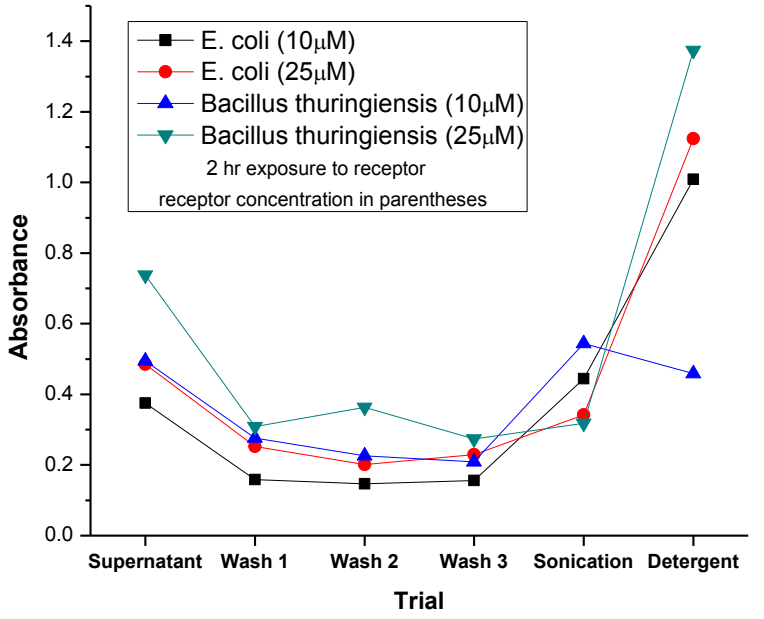
Upper: Job plot for TBAPG and **4b** (**4b** mole fraction plotted on x-axis); Bottom: Binding isotherms for the titration of **4b** with TBAPG. The JOB experiments and titration experiments were conducted at slightly different concentrations to remove any artifacts caused by different concentrations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

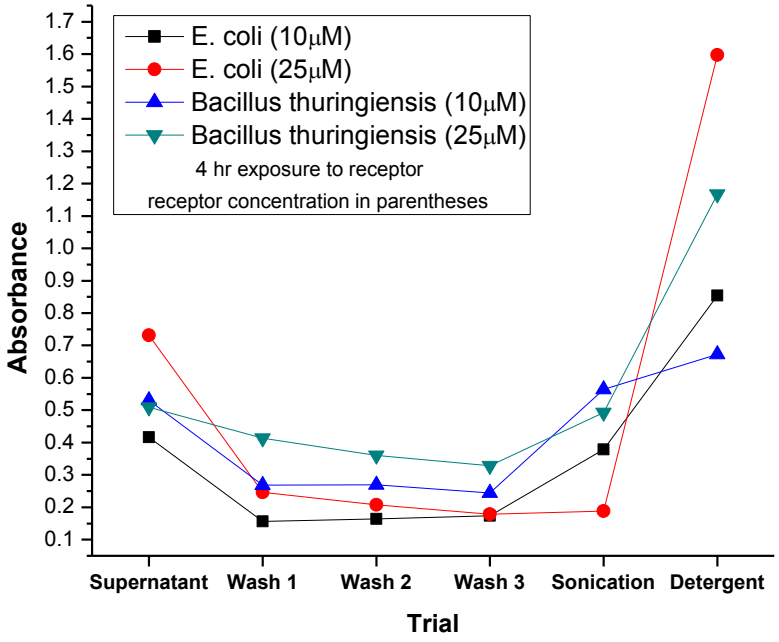




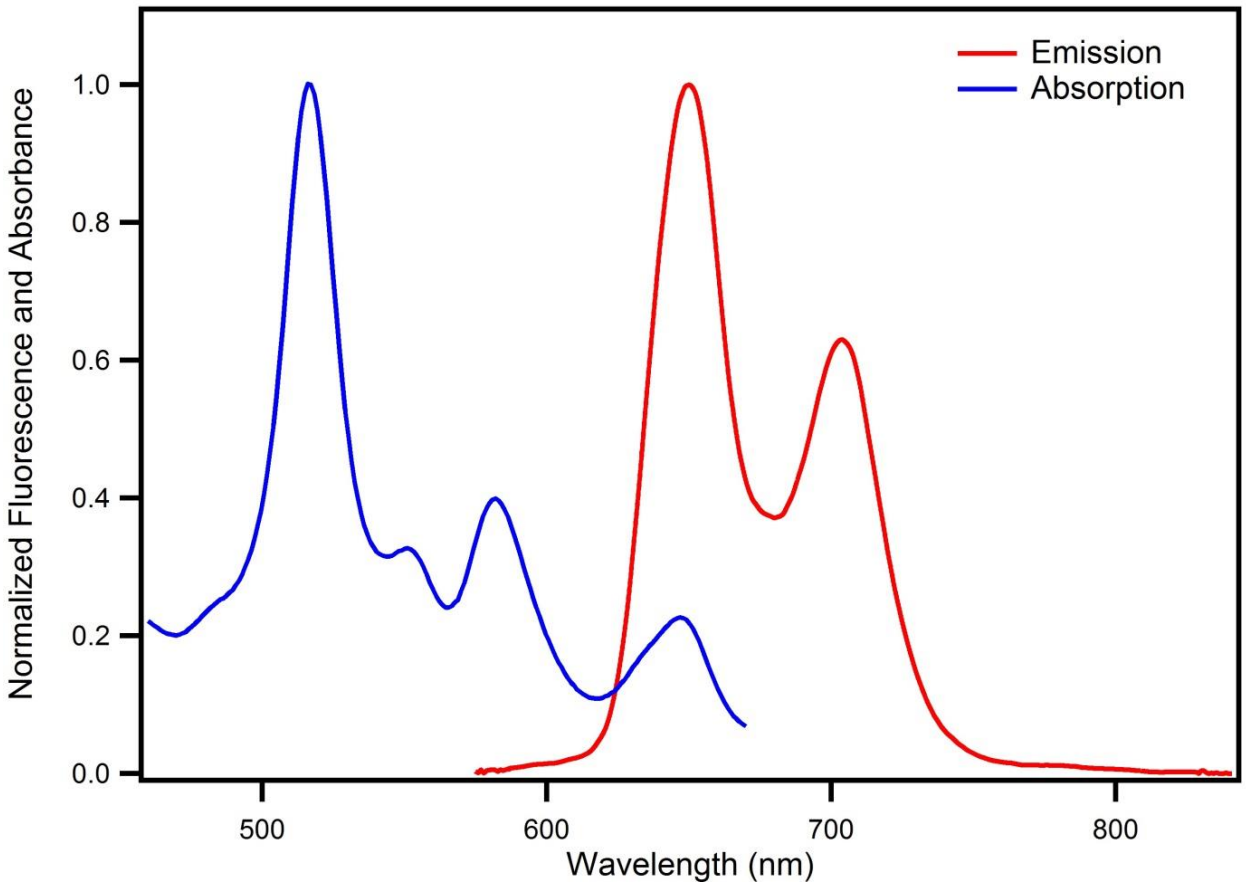


S-Figure 21: Representative example of ITC experiment in 50% DMSO/ 45% CHCl3/ 5% CH3OH at 40 ^{o}C. Upper left: ITC data for the TBAPG addition to **4b**; Upper right: ITC data for the control addition of TBAPG to solvent system; Bottom: Corrected ITC curve for the addition of TBAPG to **4b** after subtraction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





S-Figure 22: Absorbance (420 nm) of supernatants of various trials with *E. coli and Bacillus thuringensis* 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 Na_2SO_4 (50 mM) at pH 6.5.