Supporting Information

Ion-Selective Electrode Based on a Novel Biomimetic Nicotinamide Compound for Phosphate Ion Sensor

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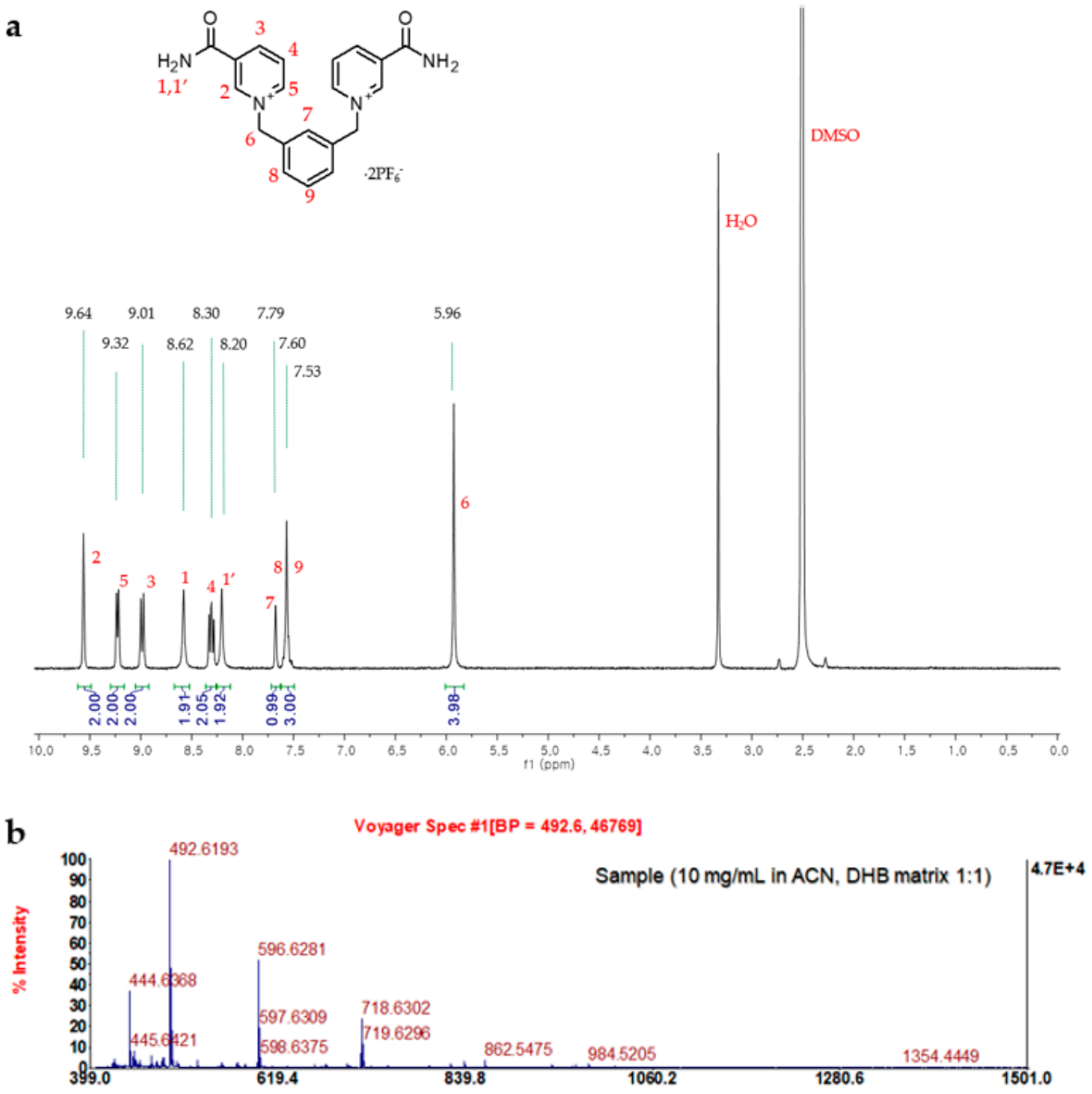


Figure S1. (a) ^{1}H-NMR spectrum of *bis-meta*-NICO-PF_6 ionophore. (b) MALDI-TOF spectrum of *bis-meta*-NICO-PF_6 m/z=492.6193 [$M^{+}PF_6^{-}$].

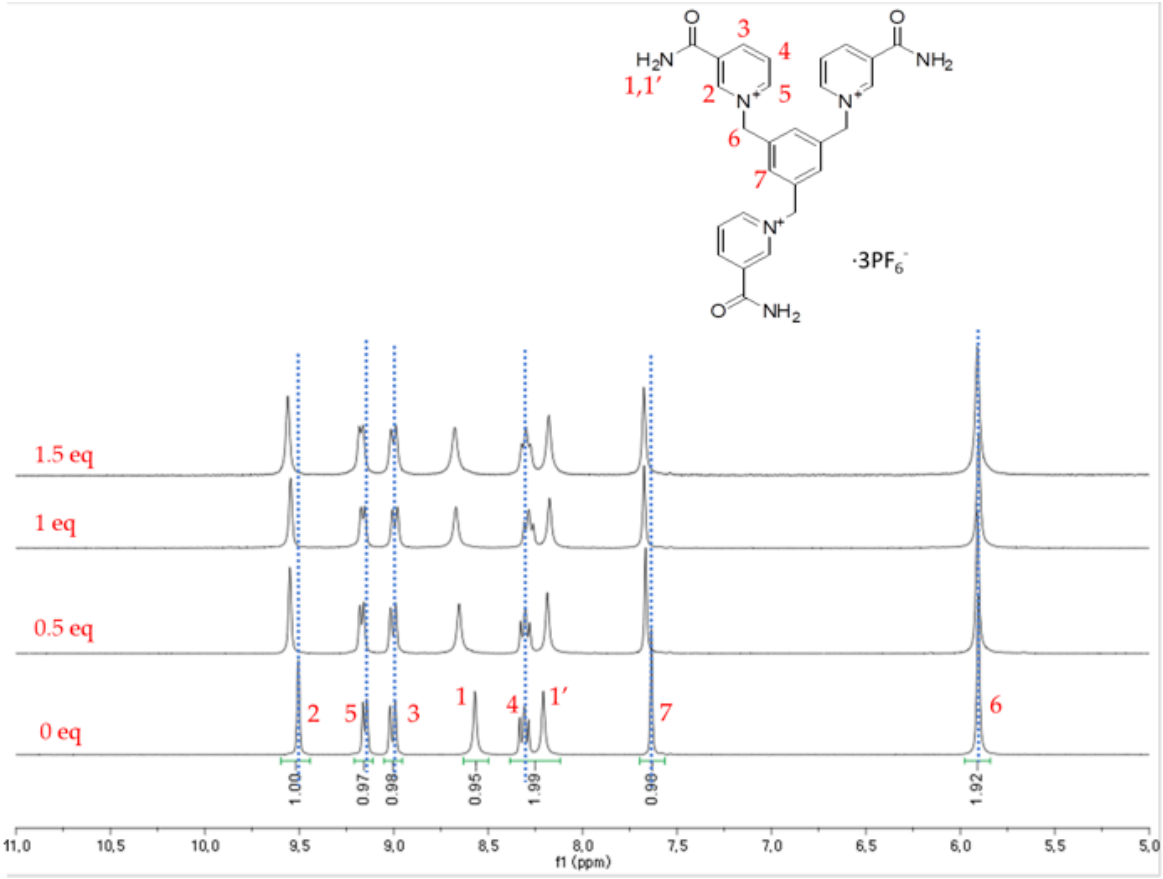


Figure S2. ^{1}H-NMR spectra of *tris-meta*-NICO-PF_6 under phosphate titration.

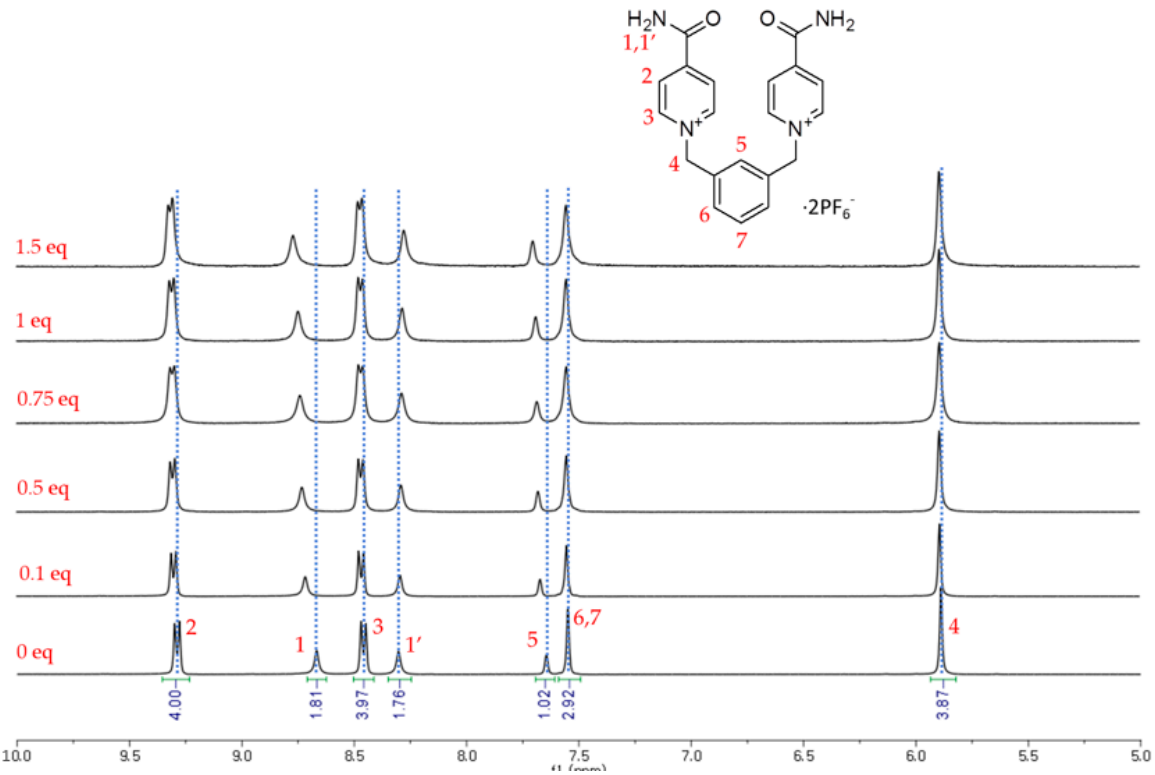


Figure S3. ^{1}H-NMR spectra of *bis-para*-NICO-PF_6 under phosphate titration study.

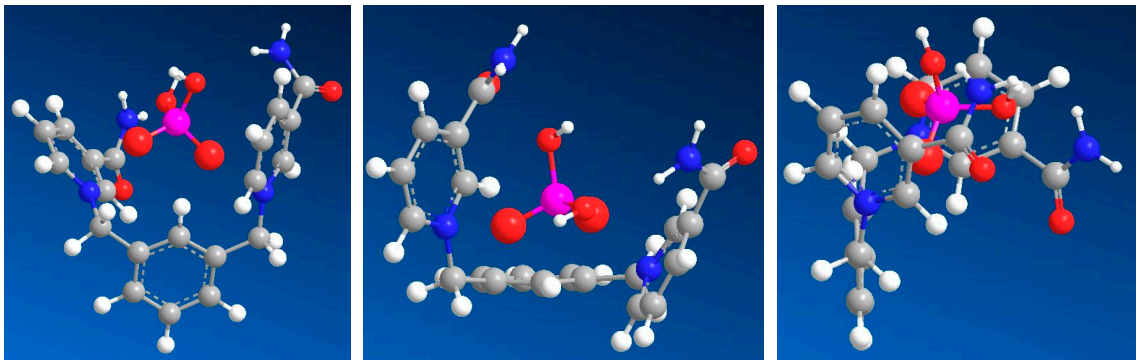


Figure S4. Three-dimensional modeling of *bis-meta*-NICO-PF_6 binding phosphate.

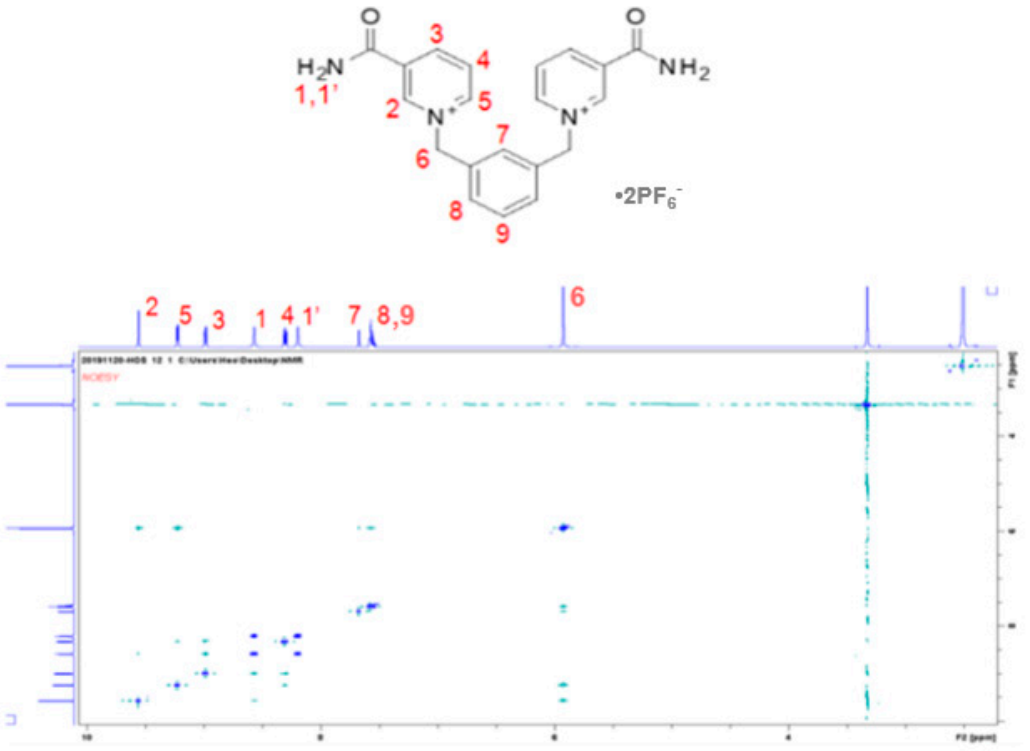


Figure S5. 2-D NOESY NMR spectrum of *bis-meta*-NICO-PF_6 .

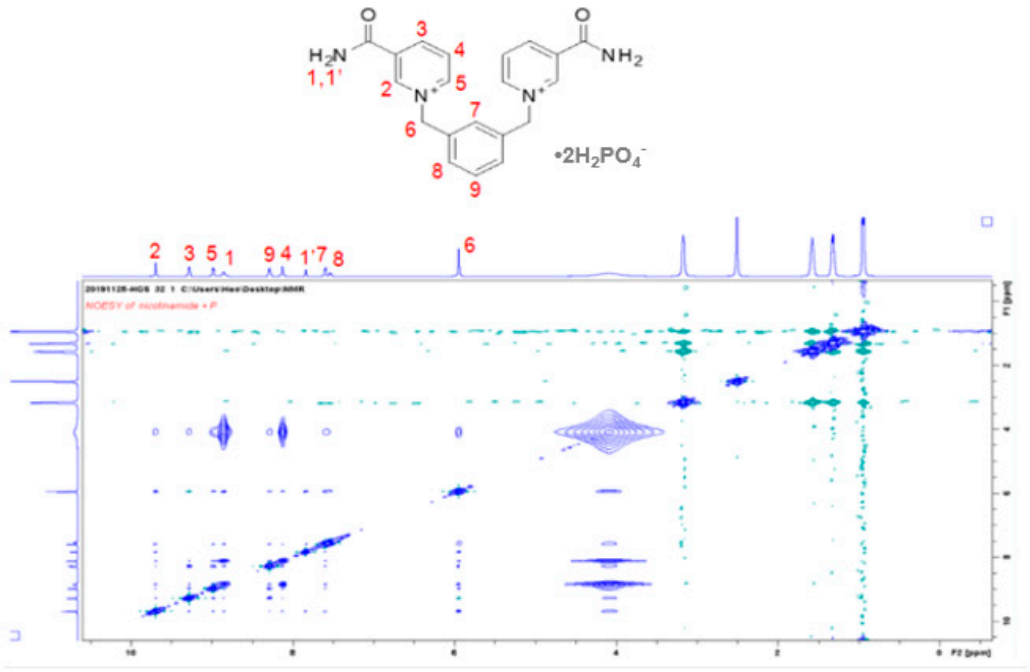


Figure S6. 2-D NOESY NMR spectrum of *bis-meta*-NICO-PF_6 with phosphate ion.

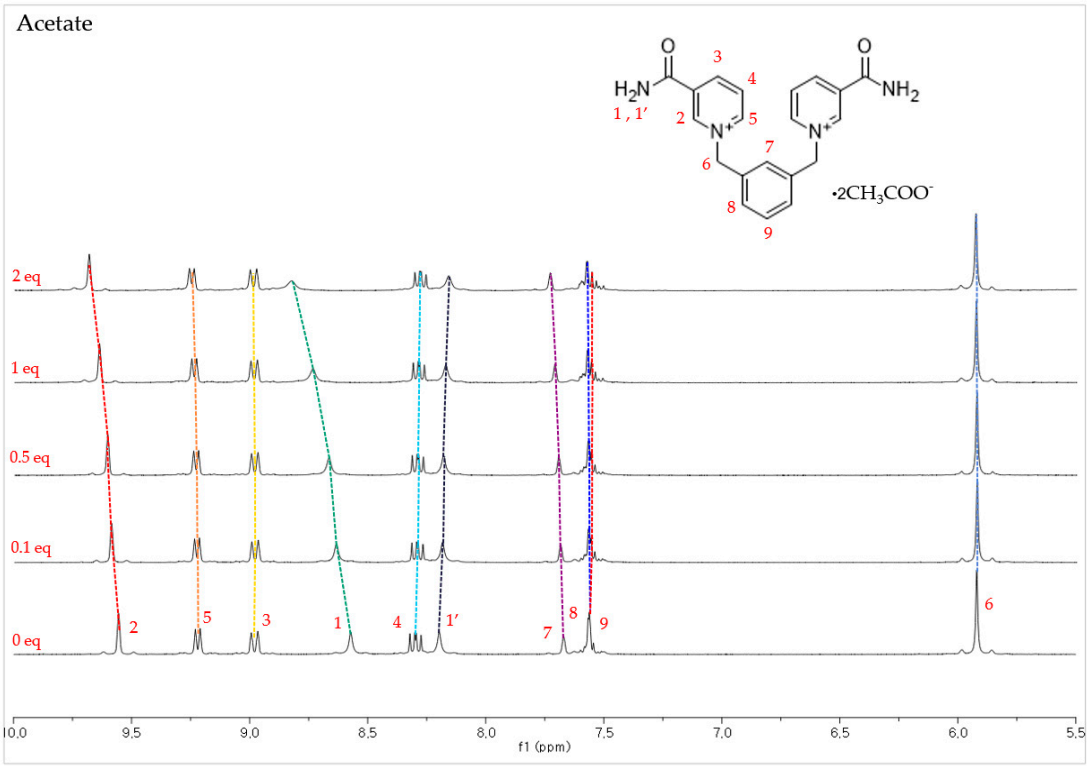


Figure S7. Acetate titration to *bis-meta*-NICO-PF_6 in DMSO-d_6.

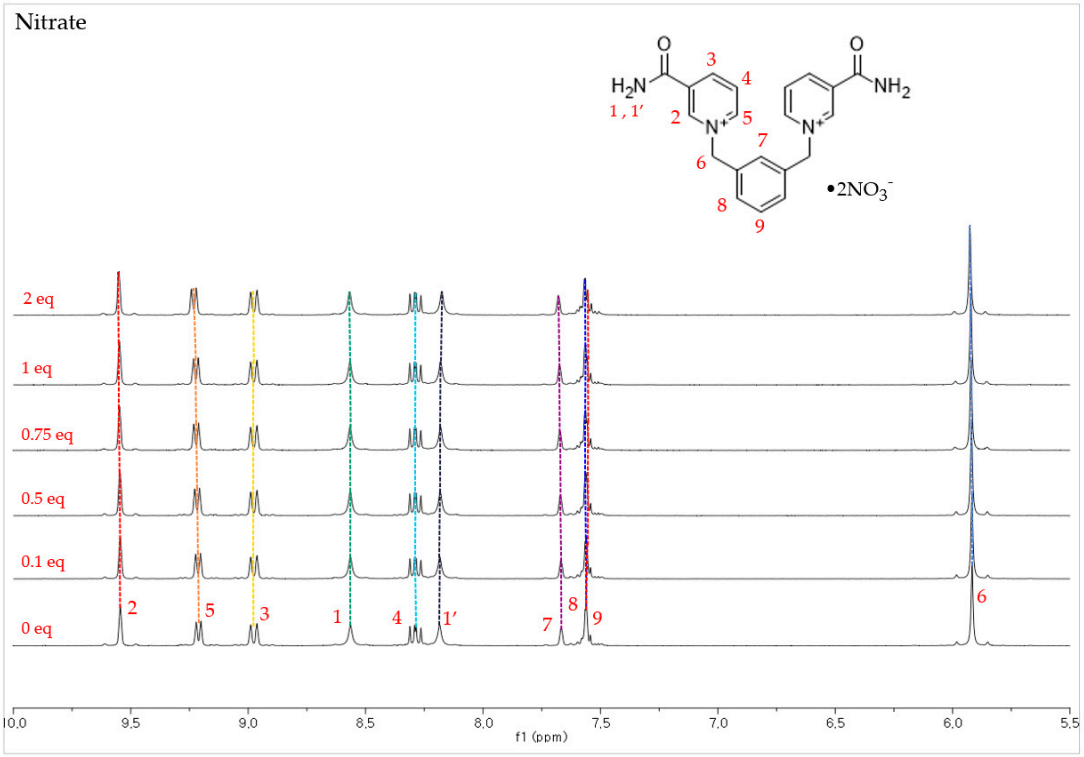


Figure S8. Nitrate titration to *bis-meta*-NICO-PF_6 in DMSO-d_6.

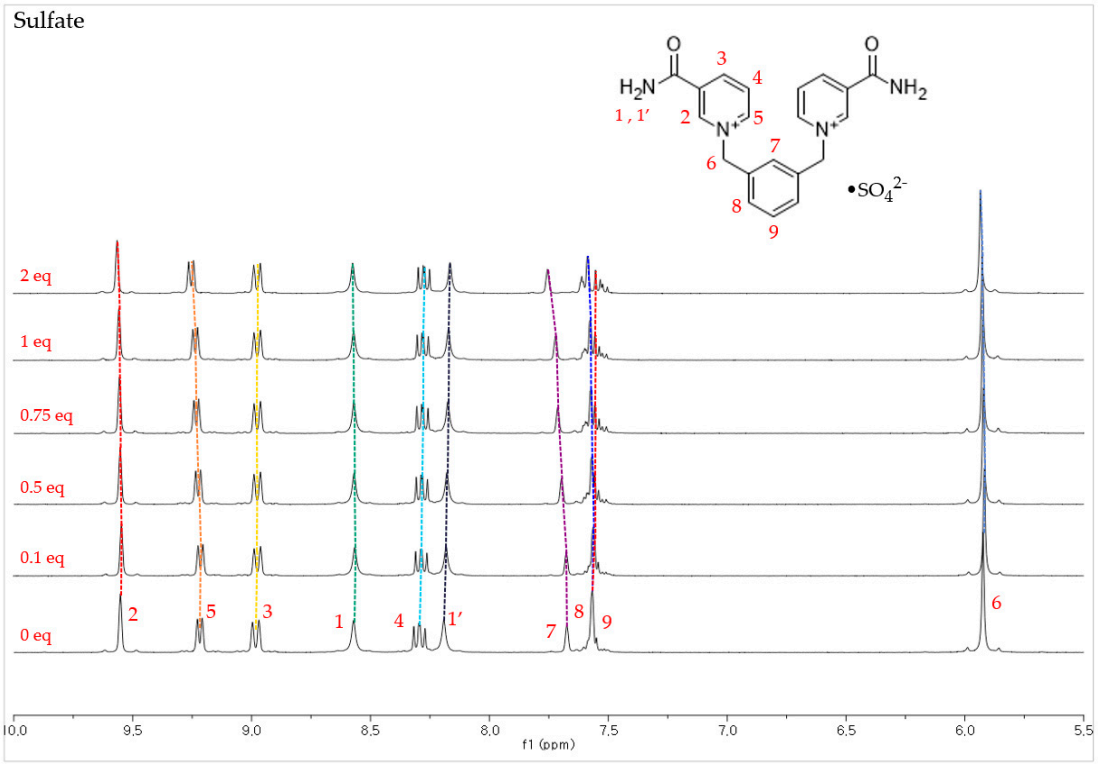


Figure S9. Sulfate titration to *bis-meta*-NICO-PF_6 in DMSO-d_6.

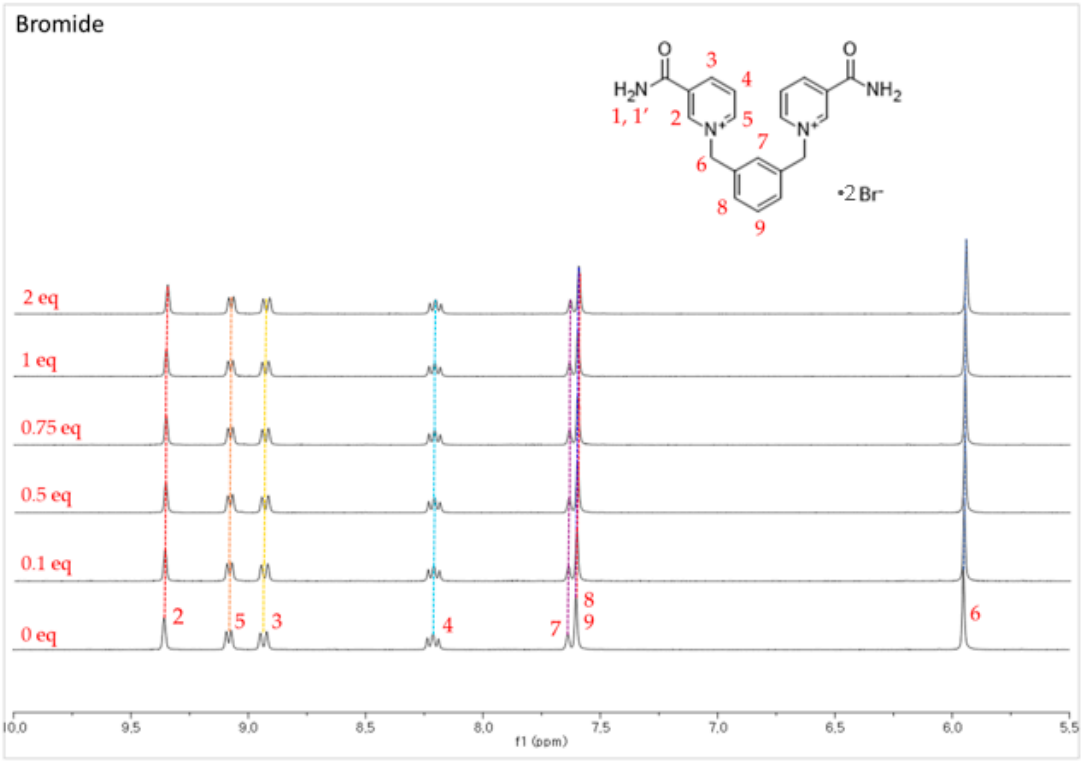


Figure S10. Bromide titration to *bis-meta*-NICO-PF_6 in DMSO-d_6.

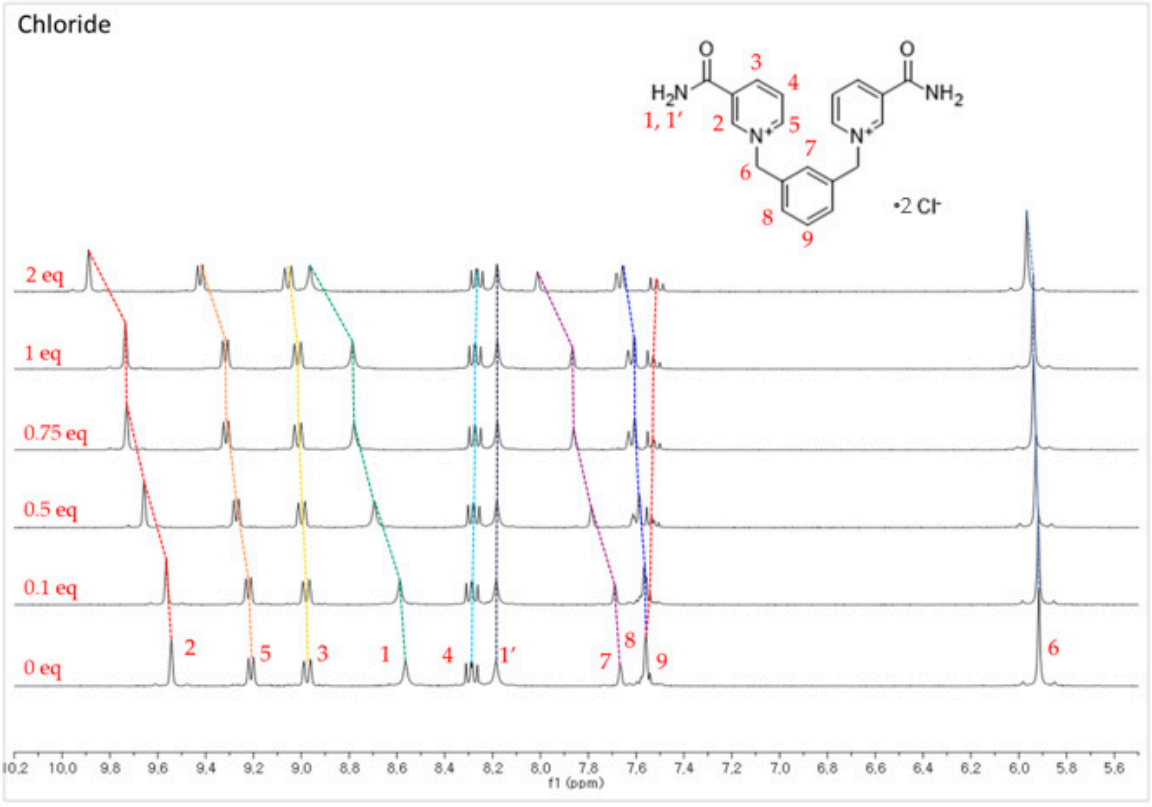


Figure S11. Chloride titration to *bis-meta*-NICO-PF_6 in DMSO-d_6.

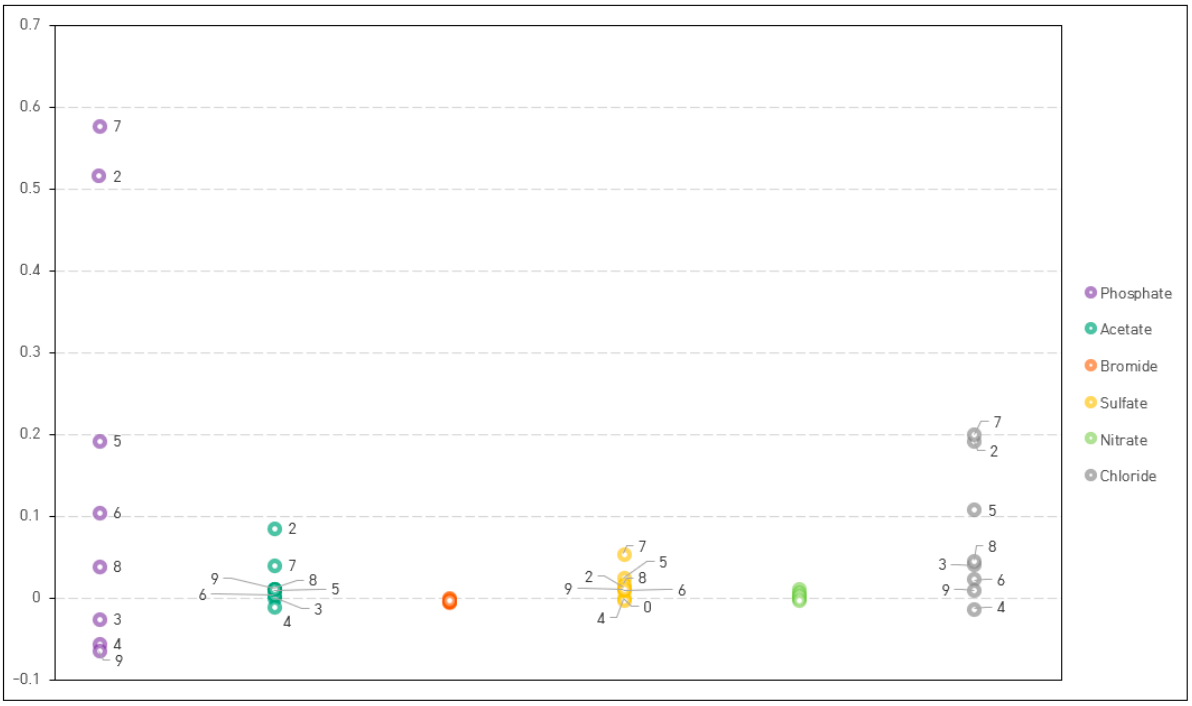


Figure S12. Chemical shift change distribution of *bis-meta*-NICO-PF_6 upon 1 equivalent of anion addition.

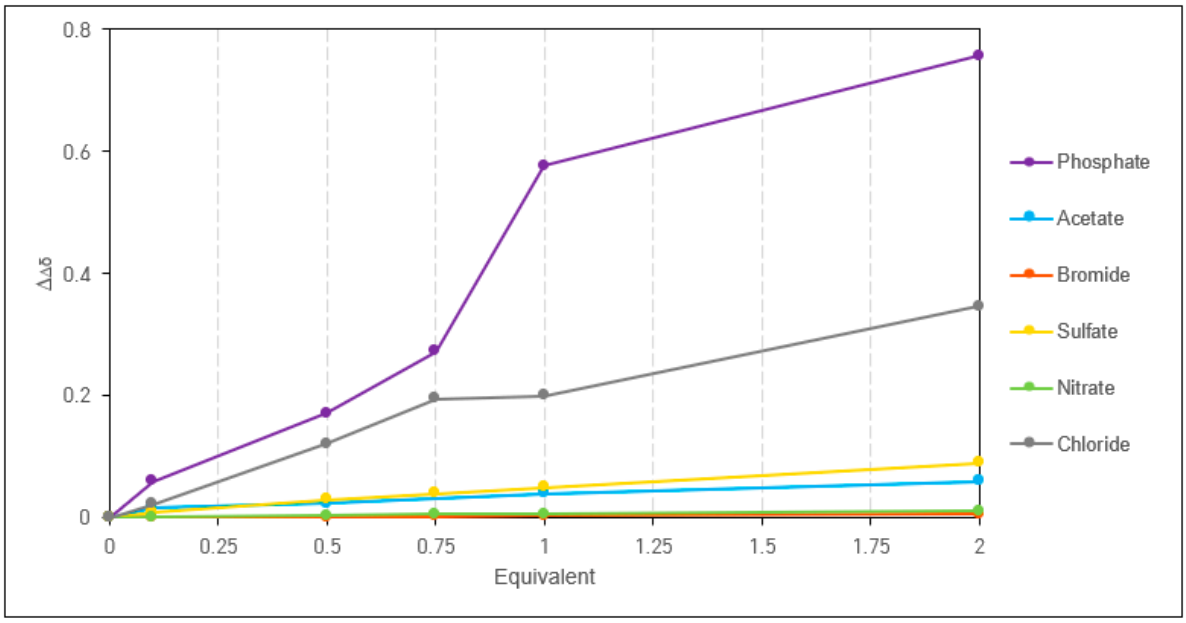
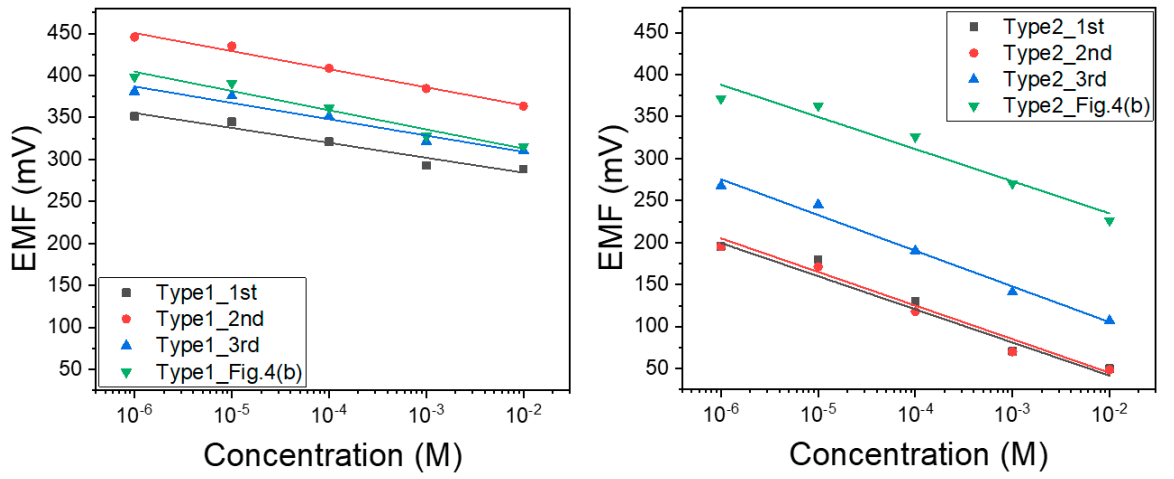


Figure S13. Chemical shift change profile of 7-H on *bis-meta*-NICO-PF_6 upon anion titration.



Type1	1st	2nd	3rd	Fig. 4(b)
Slope (mV/dec. of M)	-17.8	-21.6	-19.4	-22.9

Type2	1st	2nd	3rd	Fig. 4(b)
Slope (mV/dec. of M)	-40	-39.5	-42.5	-38.3

Figure S14. Type 1 and Type 2 ISE reproducibility across production batches.

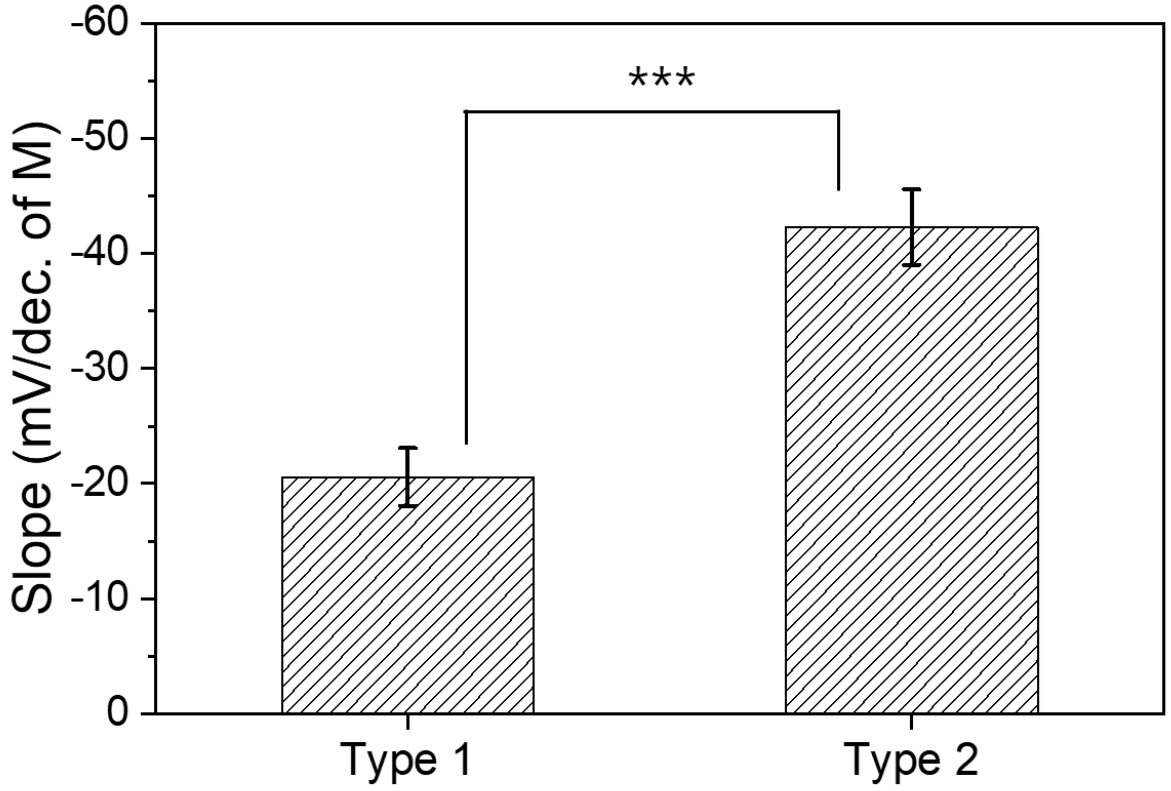


Figure S15. Slope comparison of Type 1 and Type 2 during five consecutive days. (The p-value is determined by the independent sample T verification, and the asterisk denotes the p-value, which is ***, $p < 0.001$.)