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Electronic Supplementary Information

Halogen-free Chelated Orthoborate Ionic Liquids and Organic Ionic Plastic Crystals

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CONTENT:

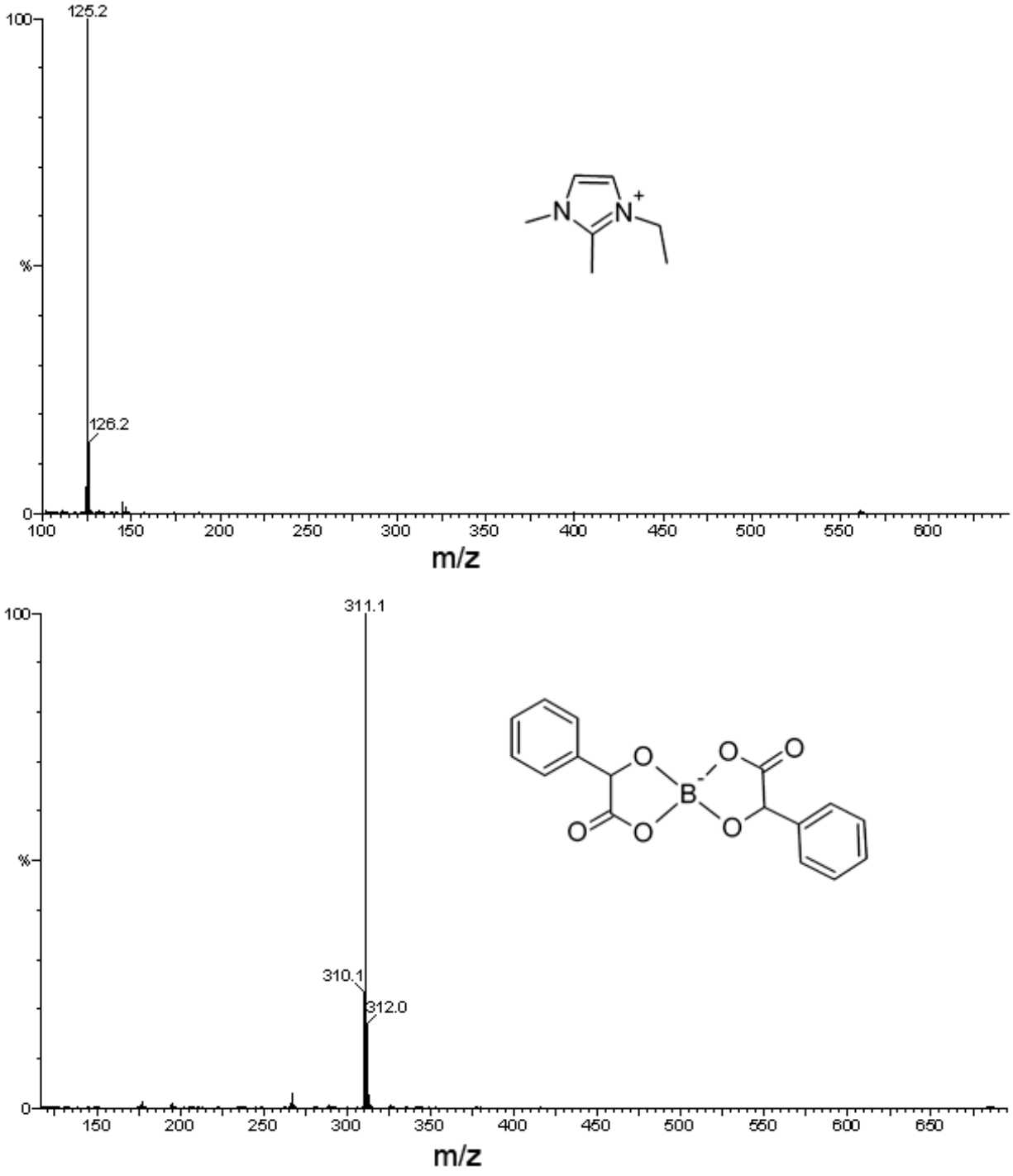

Figure SI-1. ESI-MS of [EMIm][BMB].

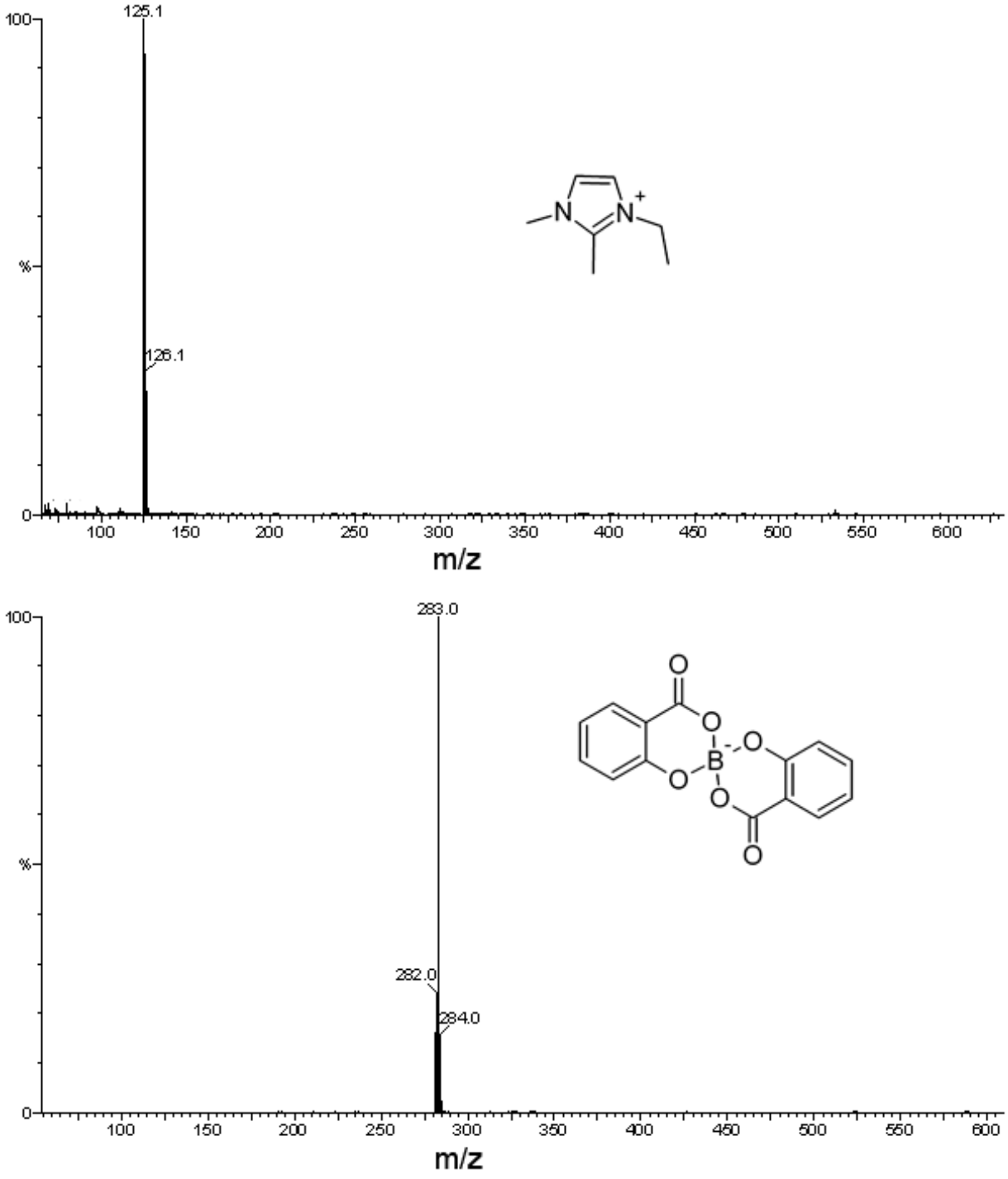

Figure SI-2. ESI-MS of [EMIm][BScB].

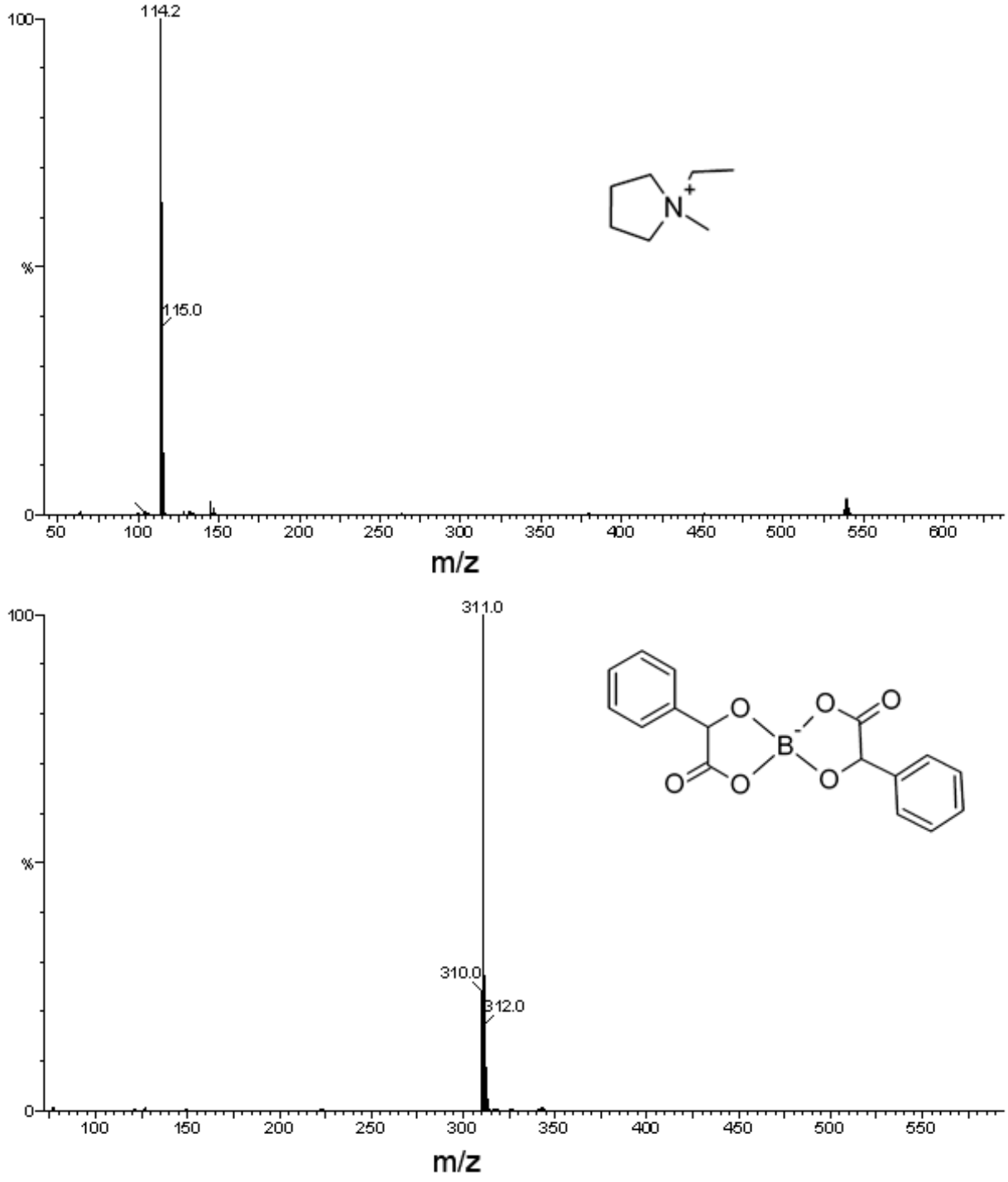

Figure SI-3. ESI-MS of [EMPy][BMB].

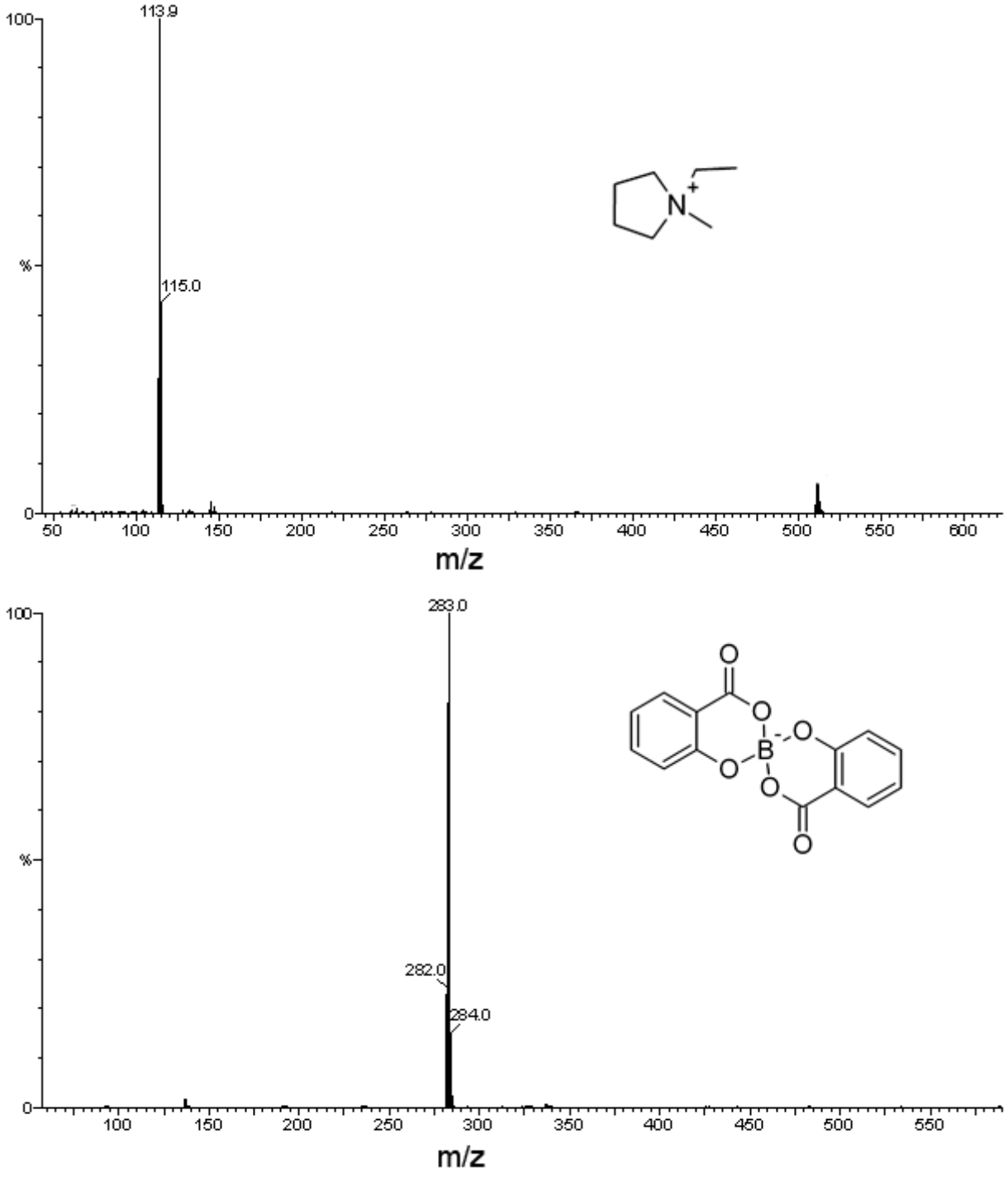

Figure SI-4. ESI-MS of [EMPy][BScB].

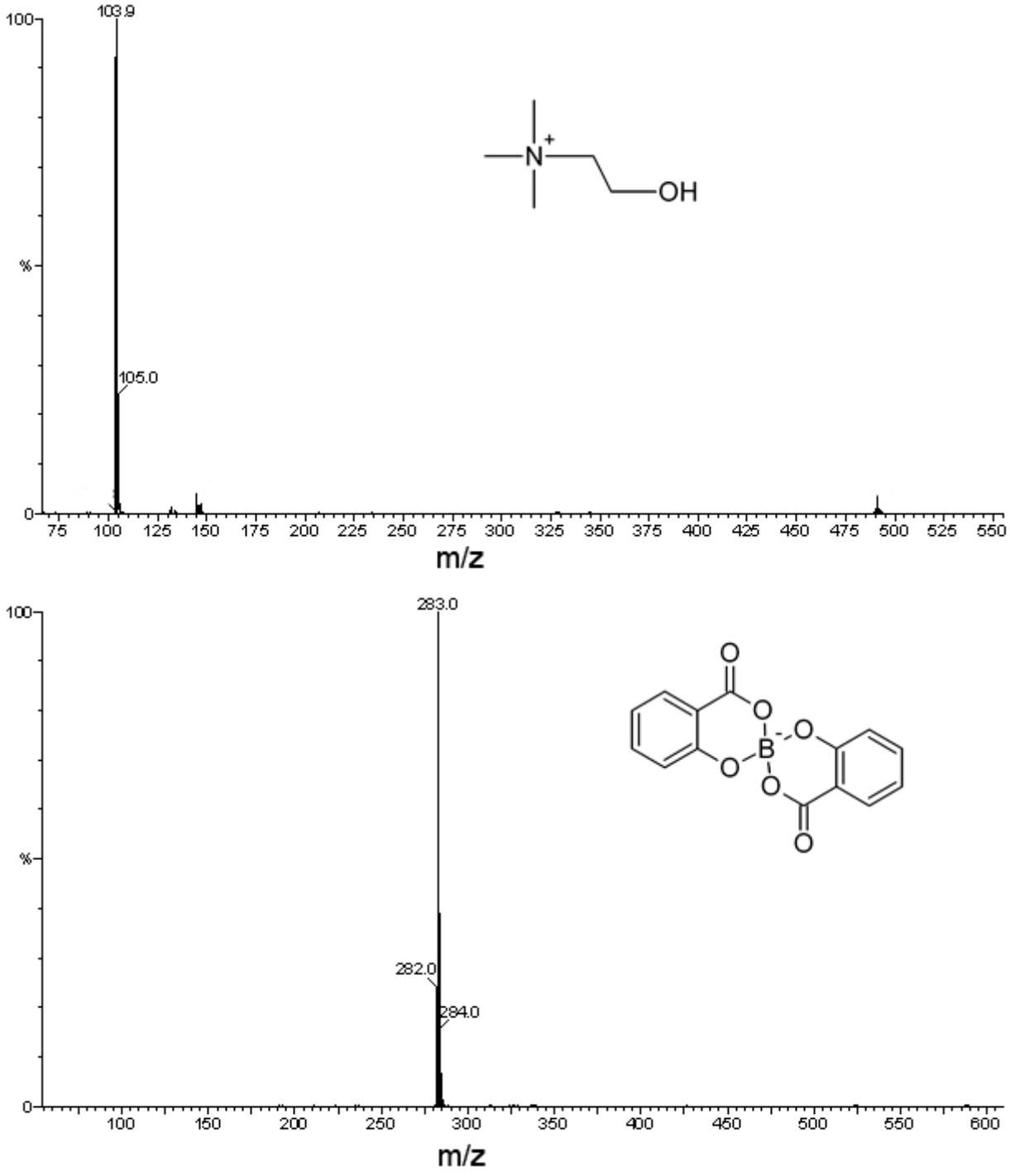

Figure SI-5. ESI-MS of [Chol][BScB].

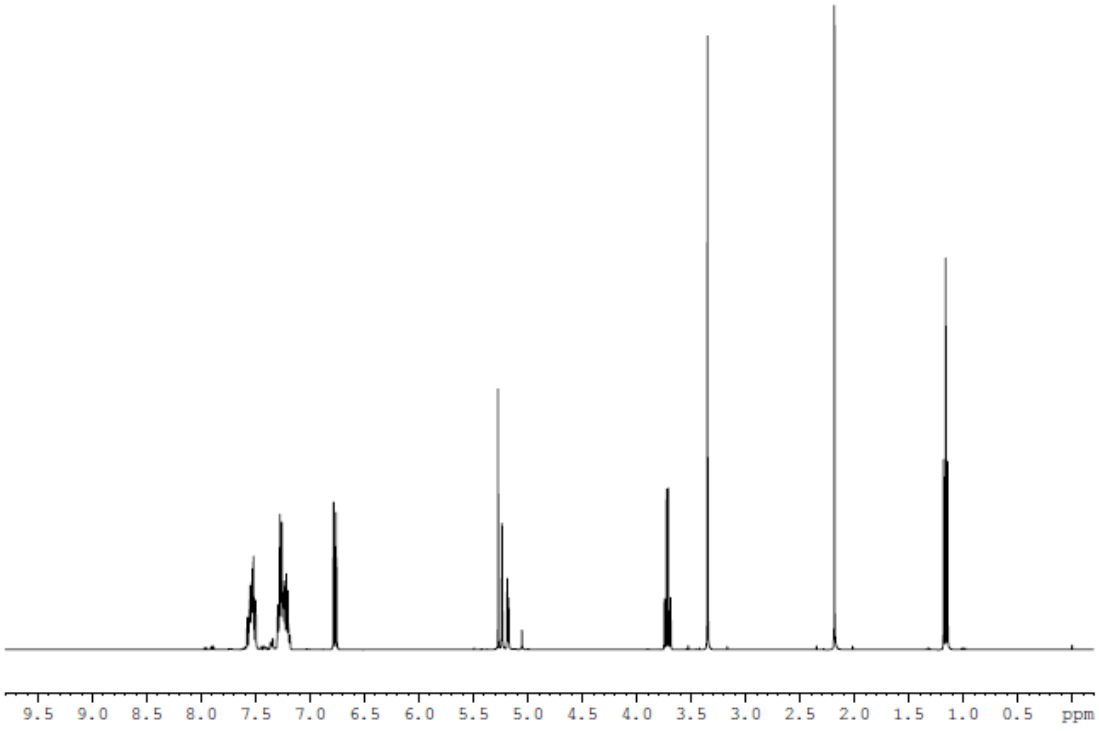

Figure SI-6. 400.17 MHz ^{1}H NMR spectrum of [EMIm][BMB] in $CDCl_3$.

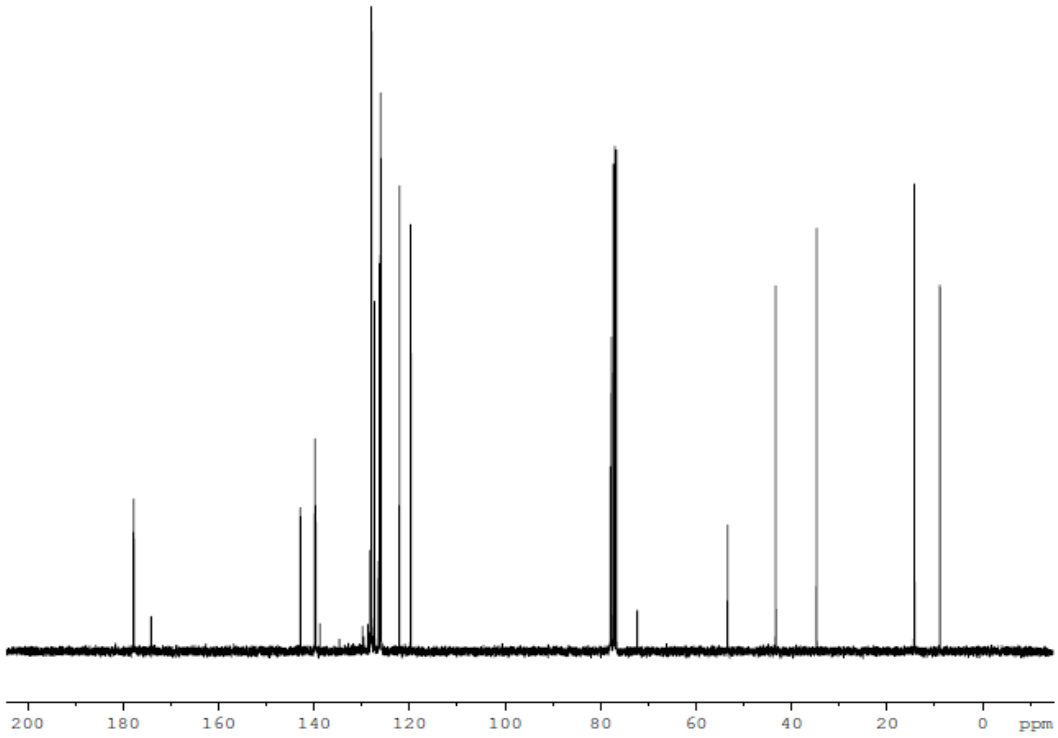

Figure SI-7. 100.63 MHz ^{13}C NMR spectrum of [EMIm][BMB] in $CDCl_3$.

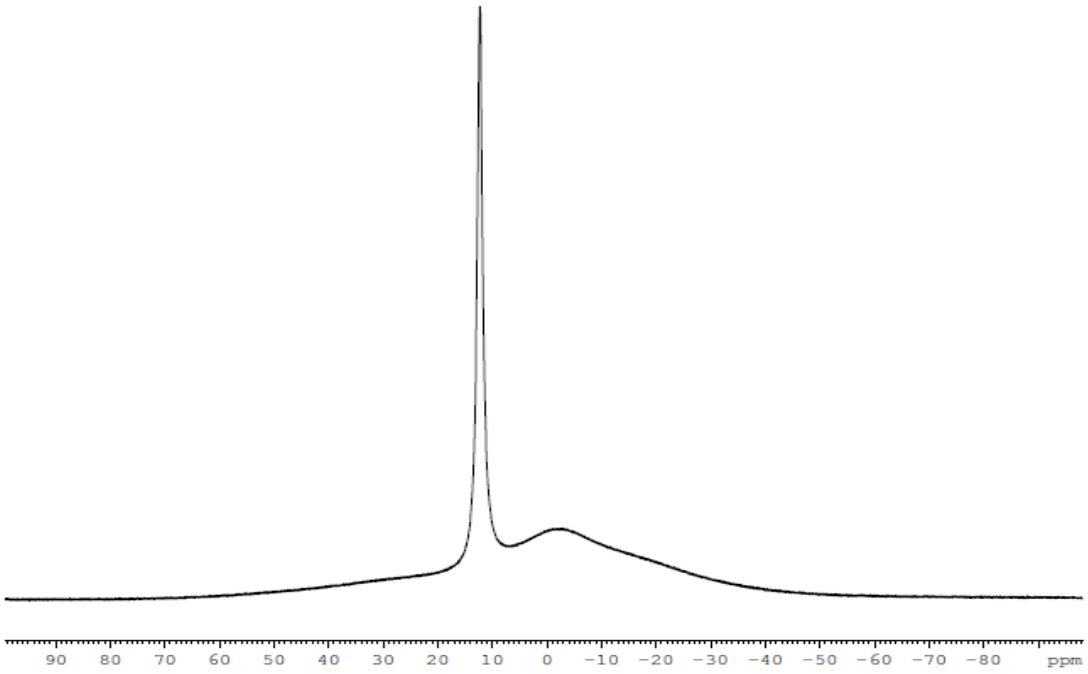

Figure SI-8. 128.39 MHz ^{11}B NMR spectrum of [EMIm][BMB] in $CDCl_3$ (A broad background signal is from the sample tube).

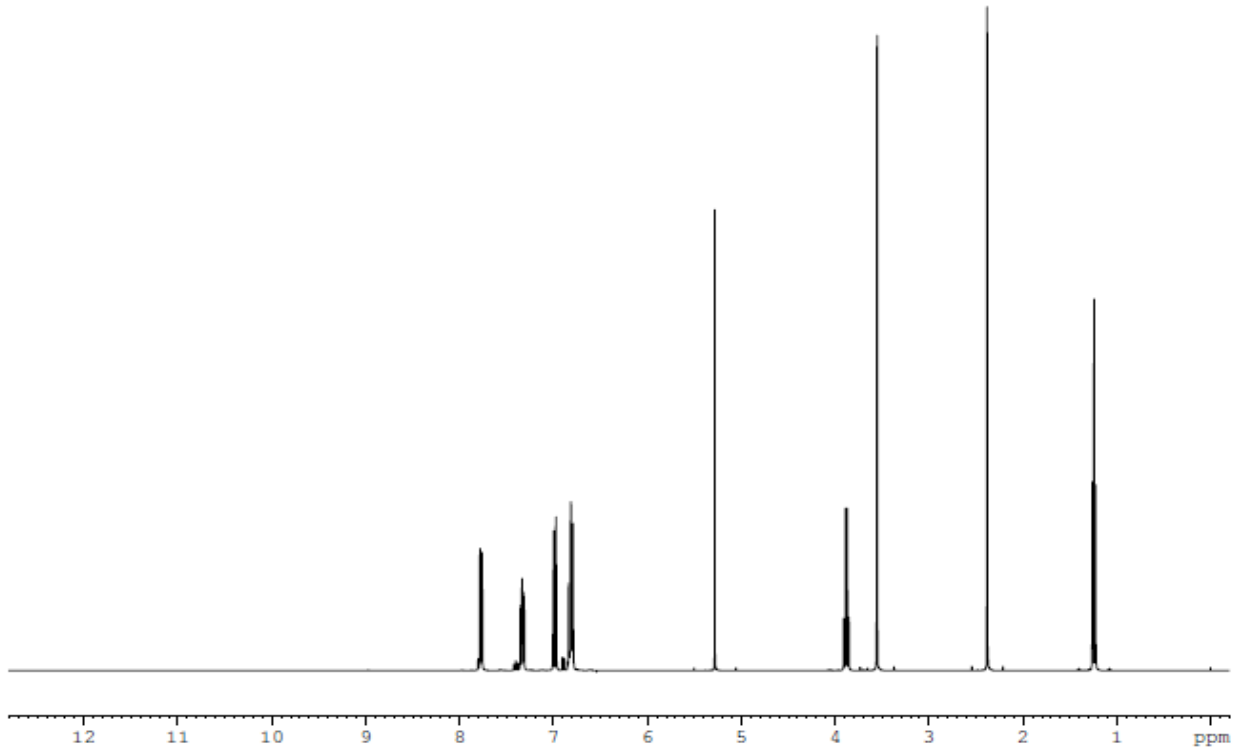

Figure SI-9. 400.17 MHz ^{1}H NMR spectrum of [EMIm][BScB] in $CDCl_3$.

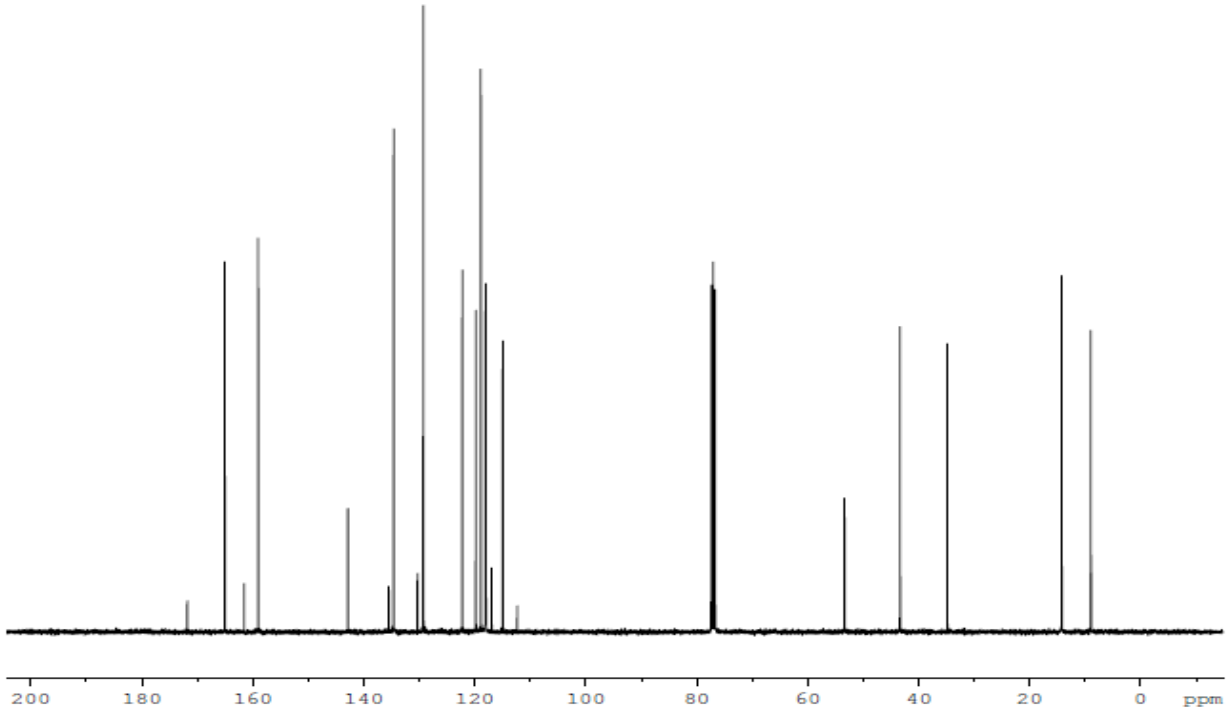

Figure SI-10. 100.63 MHz ^{13}C NMR spectrum of [EMIm][BScB] in $CDCl_3$.

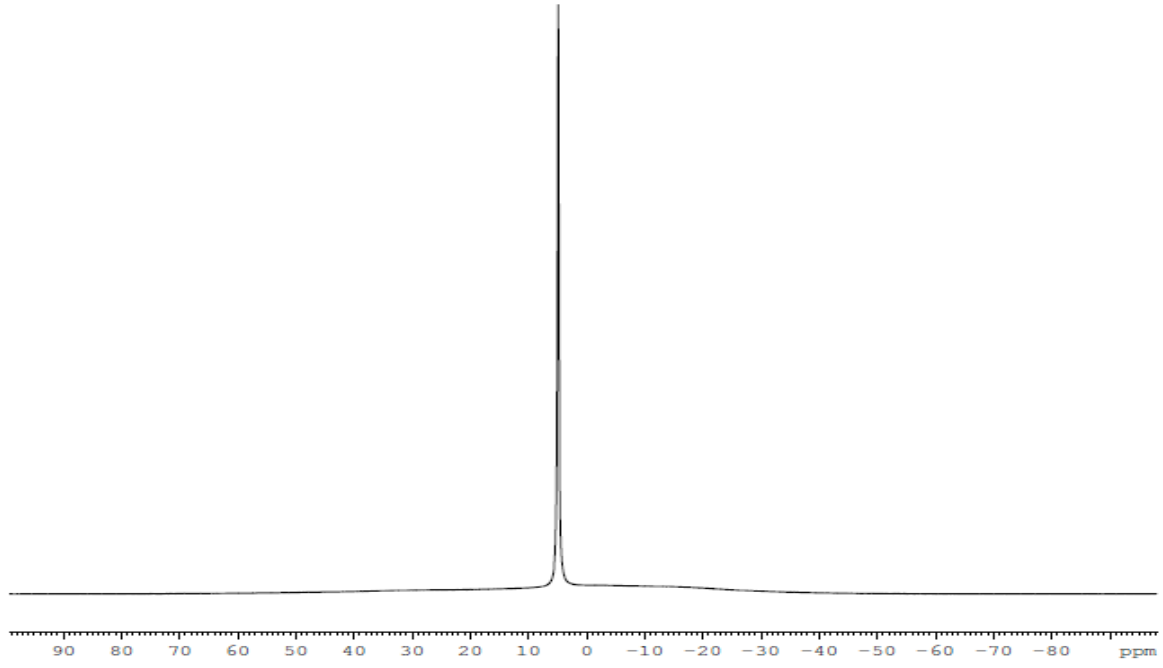

Figure SI-11. 128.39 MHz ^{11}B NMR spectrum of [EMIm][BScB] in $CDCl_3$ (A broad background signal is from the sample tube).

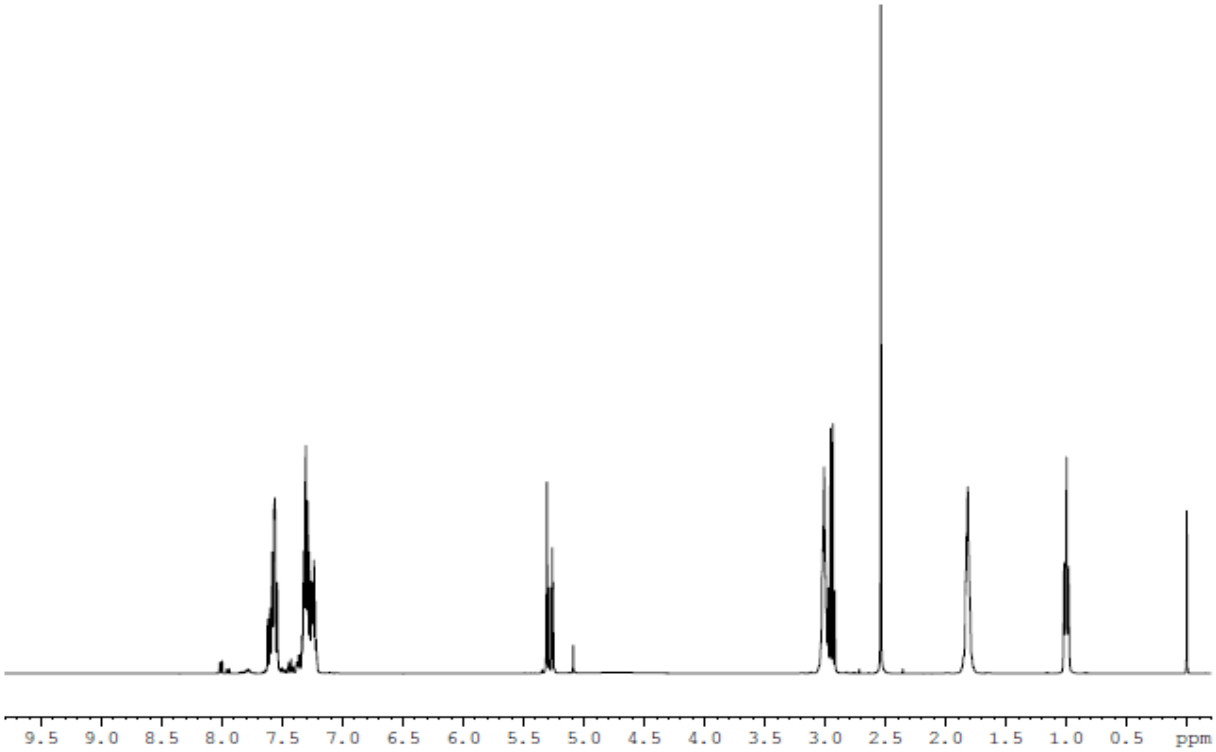

Figure SI-12. 400.17 MHz ^{1}H NMR spectrum of [EMPy][BMB] in $CDCl_3$.

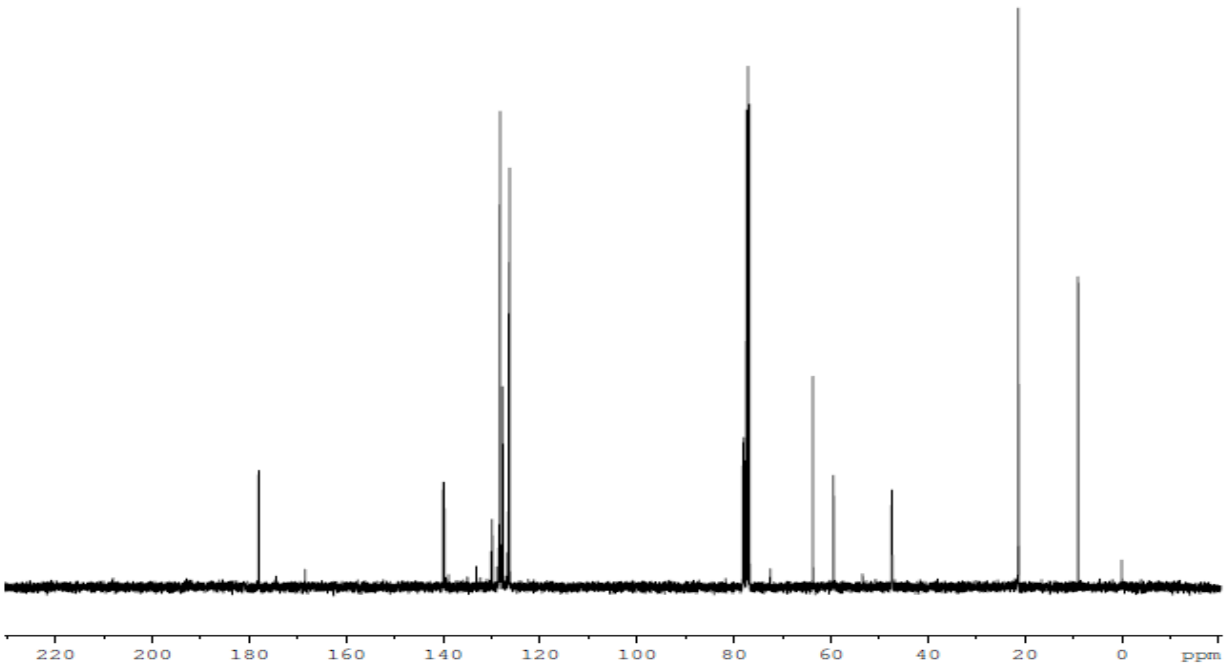

Figure SI-13. 100.63 MHz ^{13}C NMR spectrum of [EMPy][BMB] in $CDCl_3$.

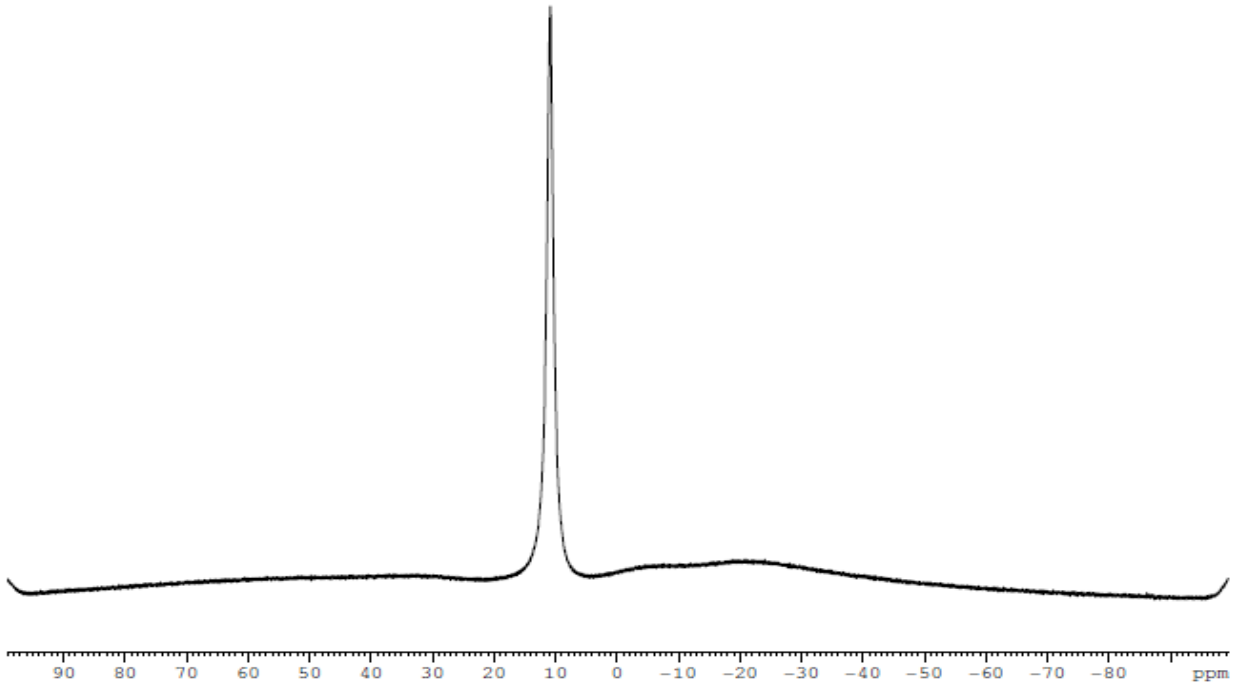

Figure SI-14. 128.39 MHz ^{11}B NMR spectrum of [EMPy][BMB] in $CDCl_3$ (A broad background signal is from the sample tube).

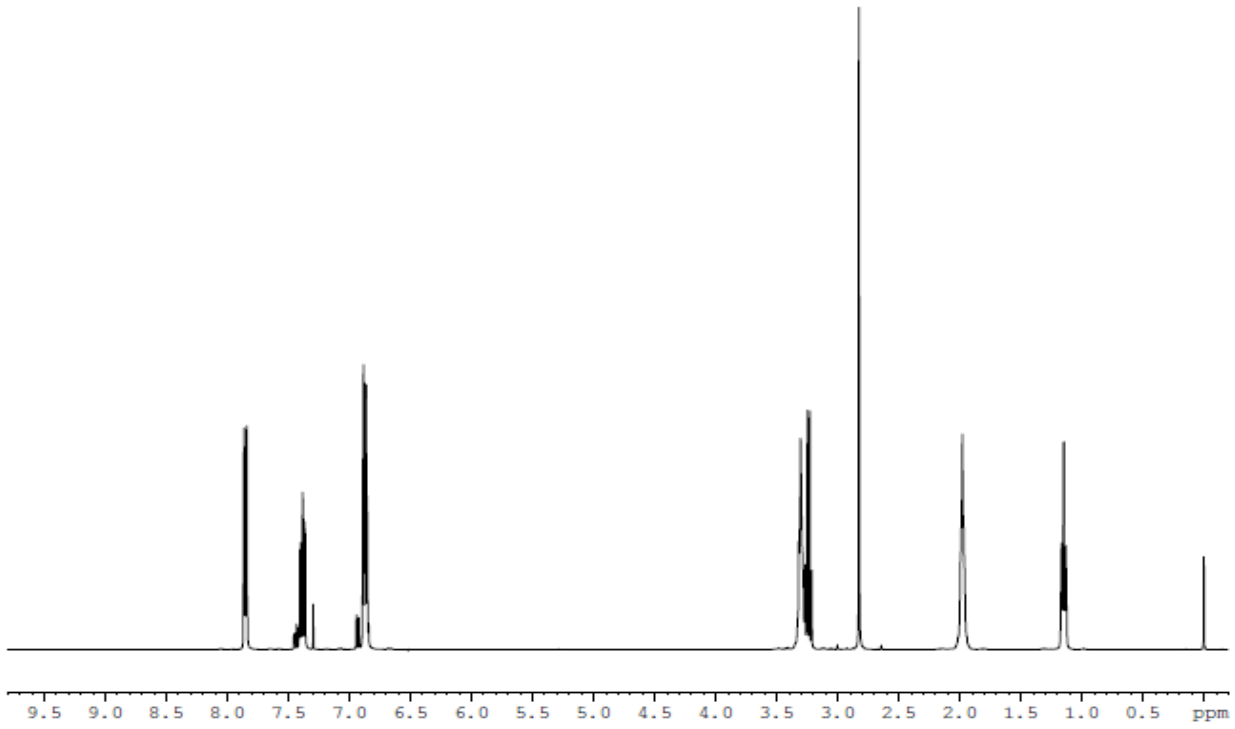

Figure SI-15. 400.17 MHz ^{1}H NMR spectrum of [EMPy][BScB] in $CDCl_3$.

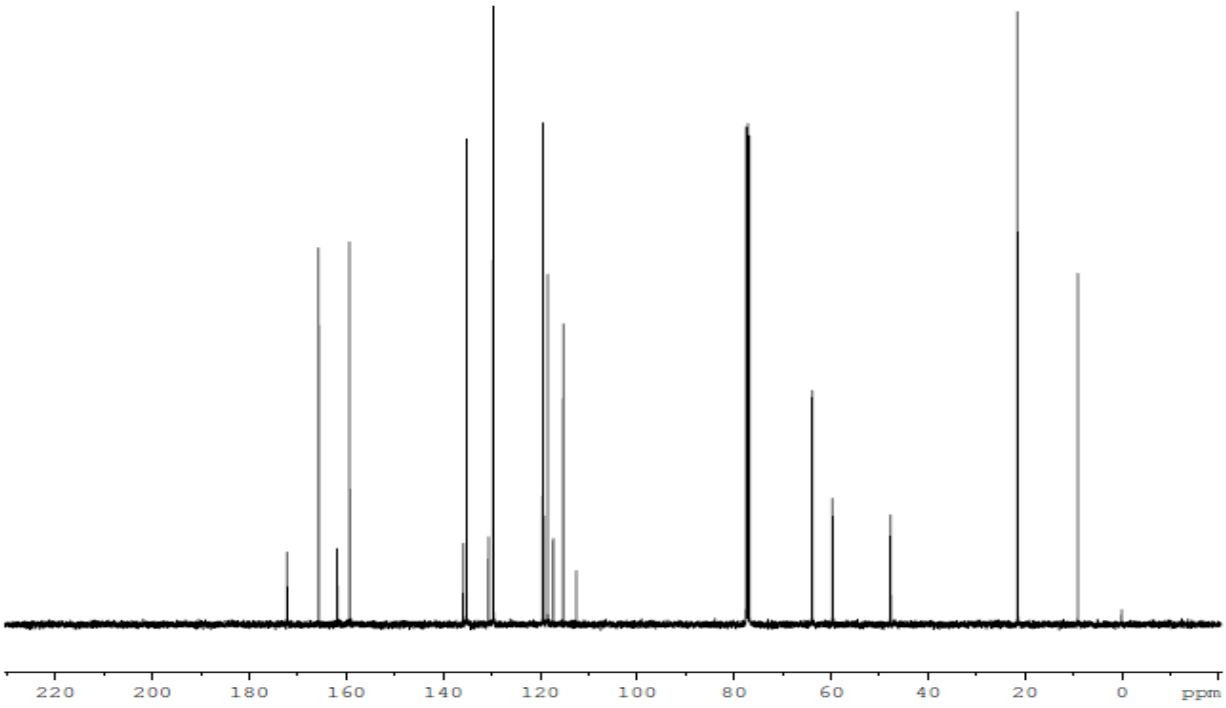

Figure SI-16. 100.63 MHz ^{13}C NMR spectrum of [EMPy][BScB] in $CDCl_3$.

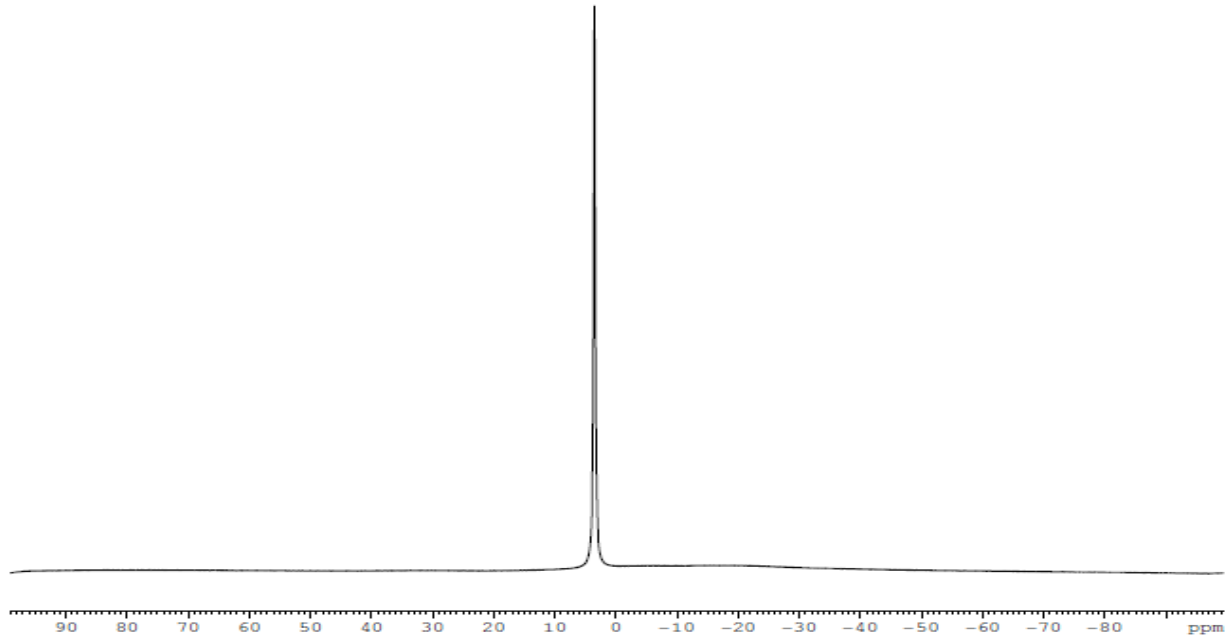

Figure SI-17. 128.39 MHz ^{11}B NMR spectrum of [EMPy][BScB] in $CDCl_3$ (A broad background signal is from the sample tube).

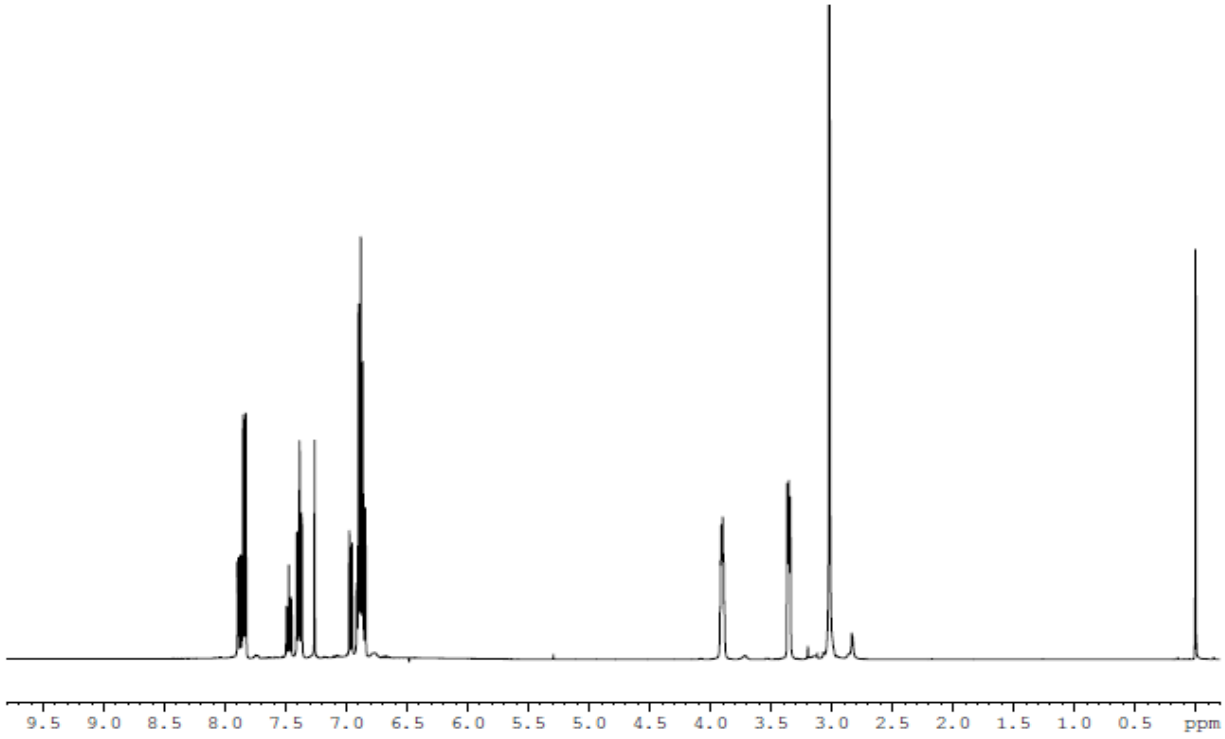

Figure SI-18. 400.17 MHz ^{1}H NMR spectrum of [Chol][BScB] in $CDCl_3$.

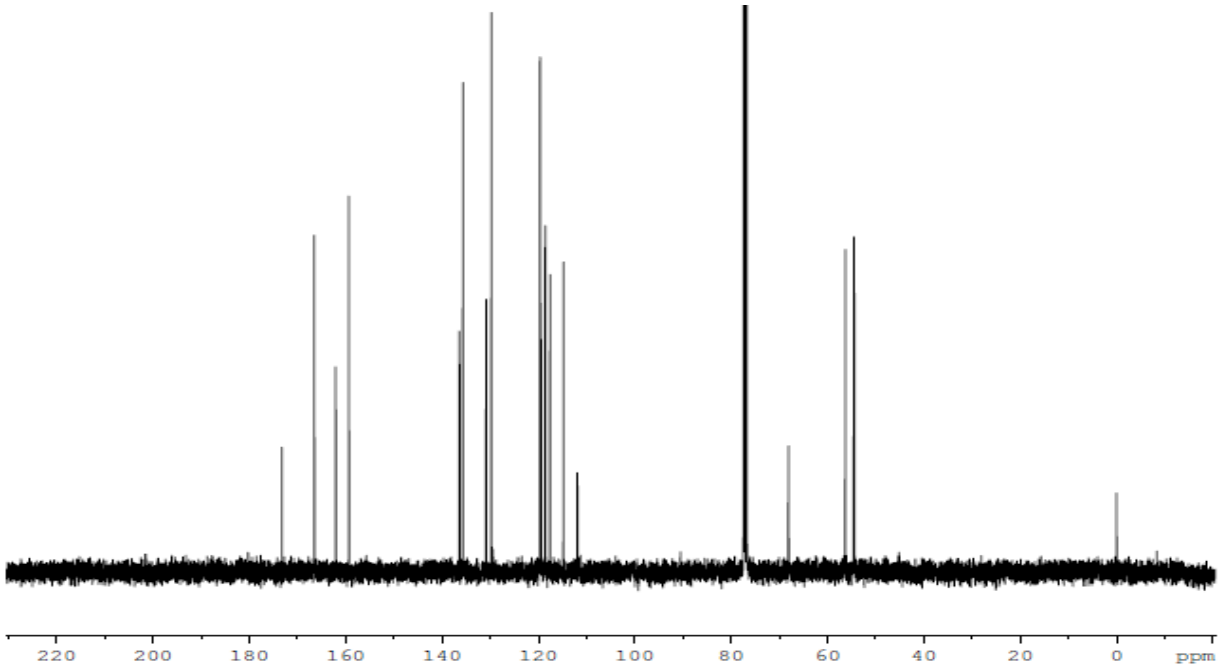

Figure SI-19. 100.63 MHz ^{13}C NMR spectrum of [Chol][BScB] in $CDCl_3$.

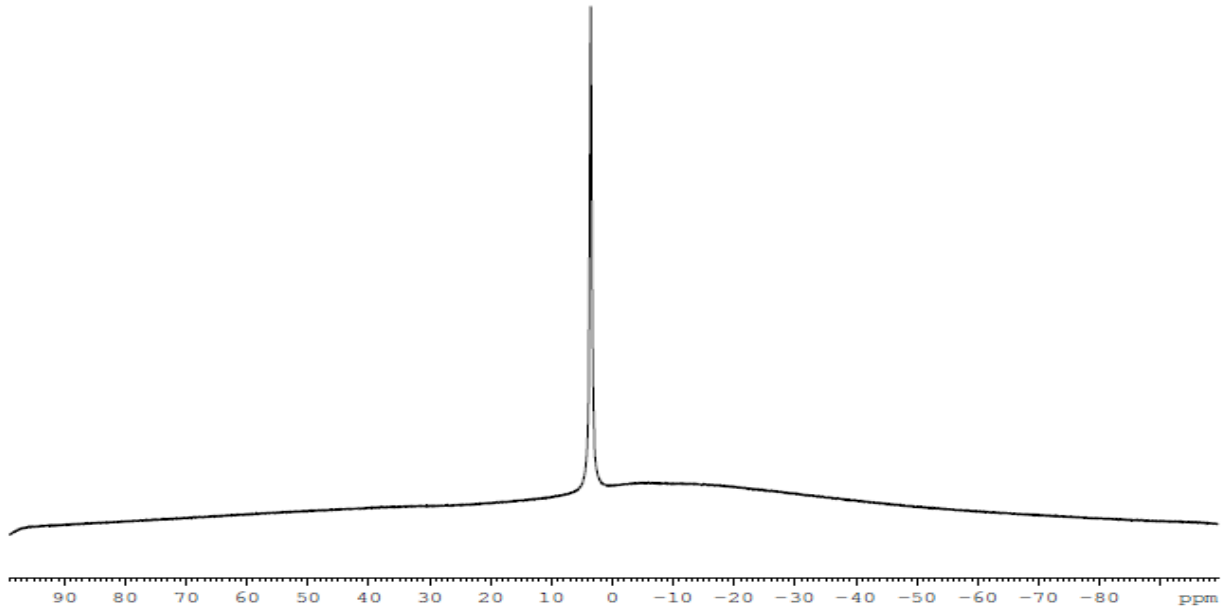

Figure SI-20. 128.39 MHz ^{11}B NMR spectrum of [Chol][BScB] in $CDCl_3$ (A broad background signal is from the sample tube).

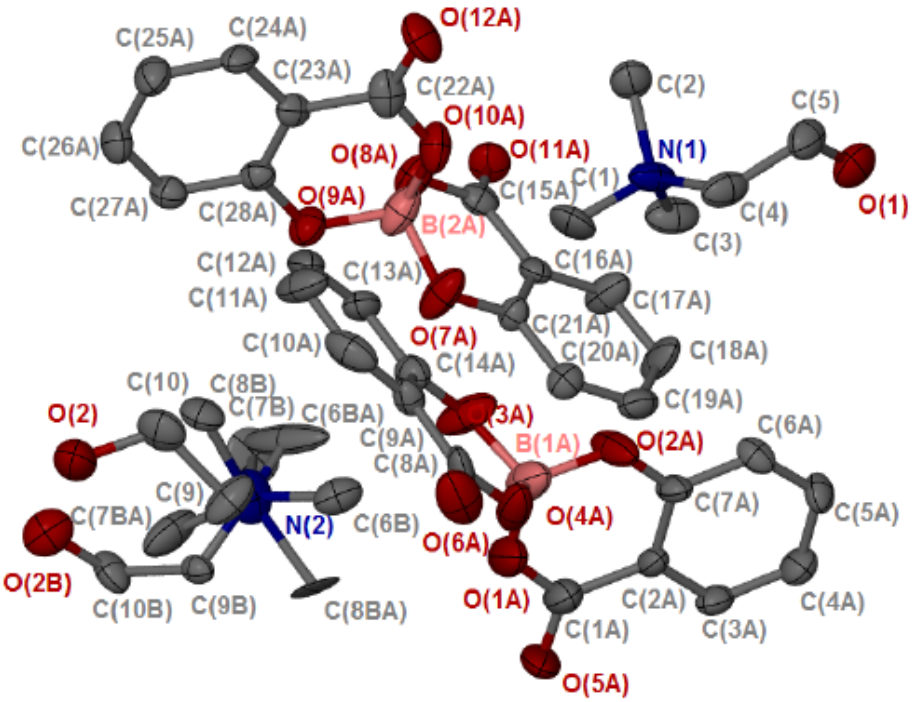

Figure SI-21. The asymmetric unit of [Chol][BScB] shown with 50 % thermal ellipsoids and the numbering scheme. The hydrogen atoms are omitted for clarity.

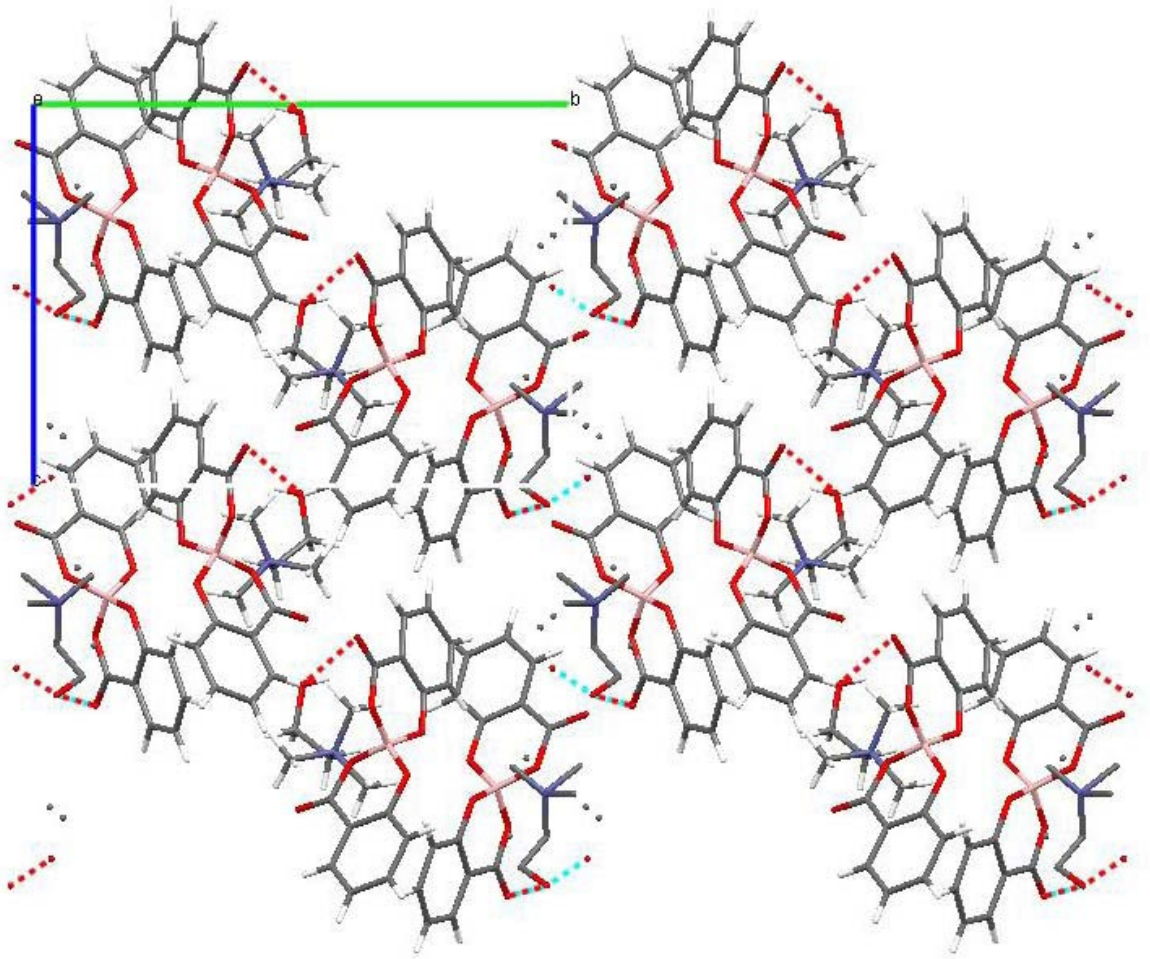

Figure SI-22. Packing diagram of [Chol][BScB] as viewed down the *a-axis* with hydrogen bonding shown in red dashed lines. The channels are clearly seen. The disordered component of the cholinium cation is shown as isolated atoms.

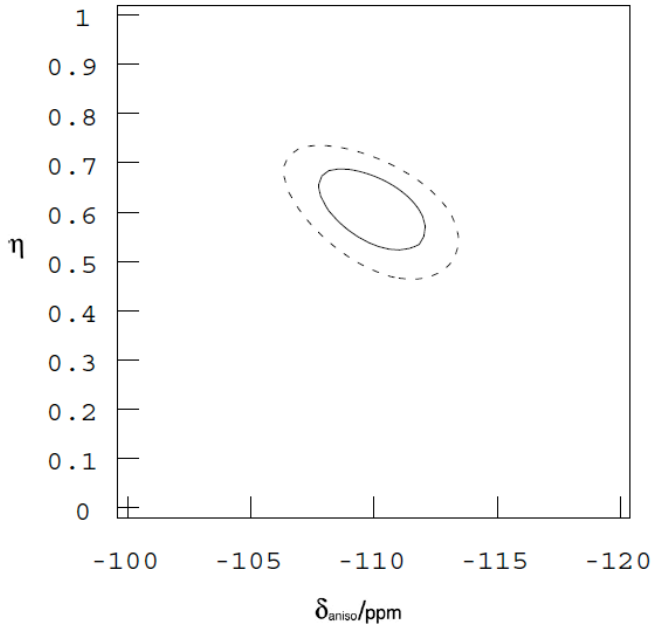

Figure SI-23. χ^2 Statistics as a function of the ^{15}N CSA parameters, δ_{aniso} and η. The plot exhibits simulations for N-sites of [EMIm][BScB] with isotropic chemical shift 142.8 ppm. The 68.3% joint confidence limit (solid line) and 95.4% joint confidence limit (dashed line) for the two CSA parameters are shown.

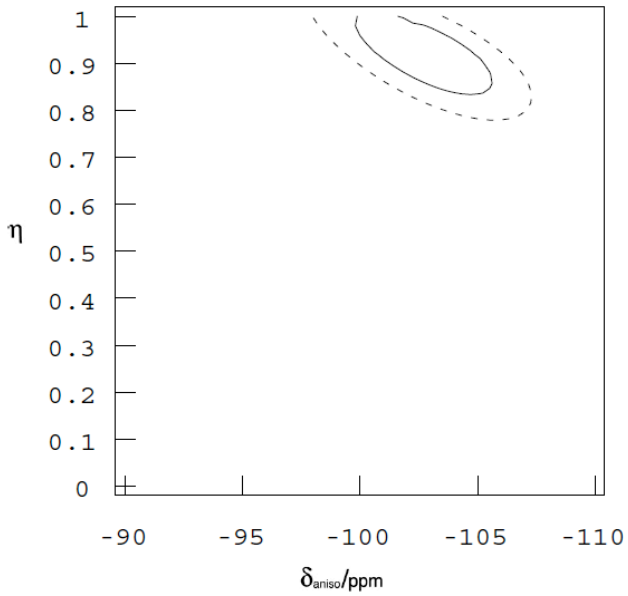

Figure SI-24. χ^2 Statistics as a function of the ^{15}N CSA parameters, δ_{aniso} and η. The plot exhibits simulations for N-sites of [EMIm][BScB] with isotropic chemical shift 131.3 ppm. The 68.3% joint confidence limit (solid line) and 95.4% joint confidence limit (dashed line) for the two CSA parameters are shown.

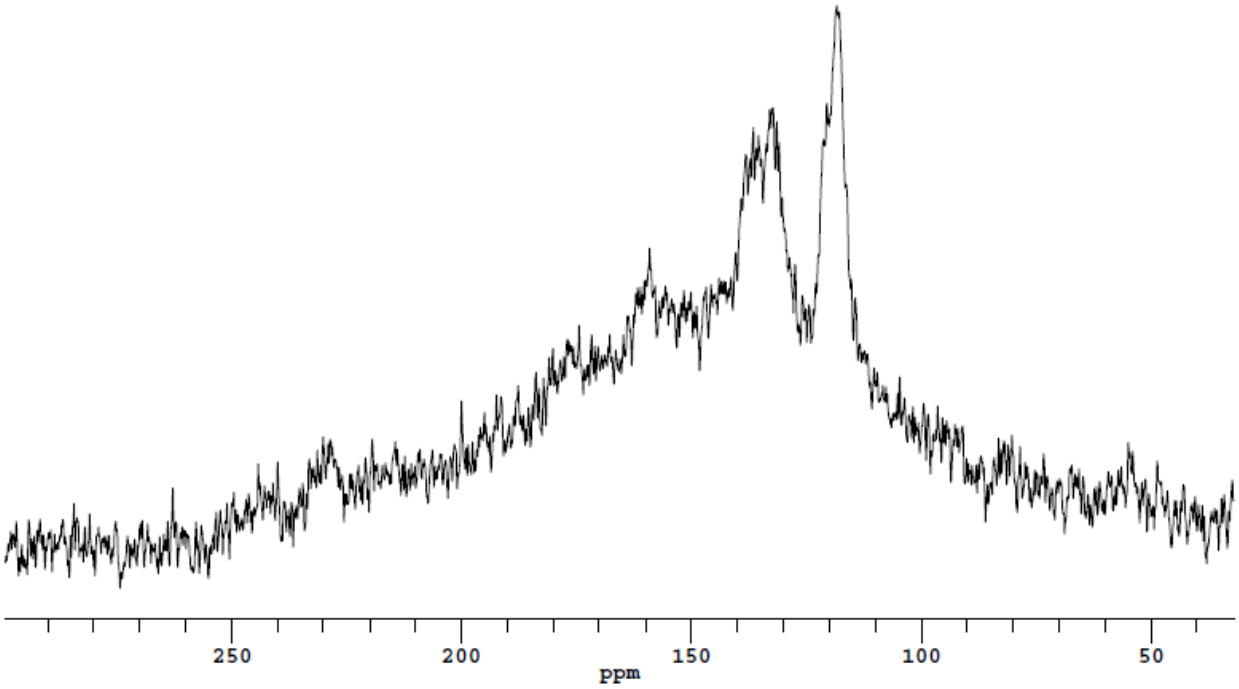

Figure SI-25. ^{13}C CP/MAS NMR spectrum of a powder lanthanum complex with bis(salicylato)borate after the extraction process of La^{3+}(aq) by [Chol][BScB]. Resonance lines between 120 and 140 ppm are assigned to aromatic carbon sites in the salicylic groups of the complex. Resonance lines at 230-250 ppm are spinning sidebands.