

Supporting Information

Enhanced In Vitro Antiviral Activity of Hydroxychloroquine Ionic Liquids Against SARS-CoV-2

FTIR spectra

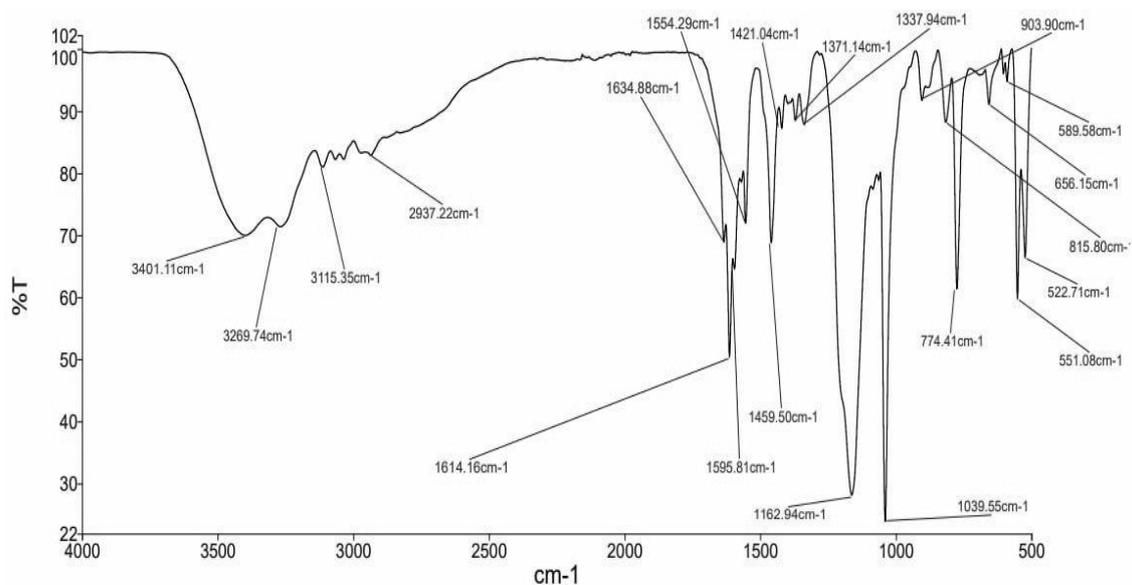


Figure S1. FTIR-ATR spectrum of [HCQH₂][C₁SO₃]₂.

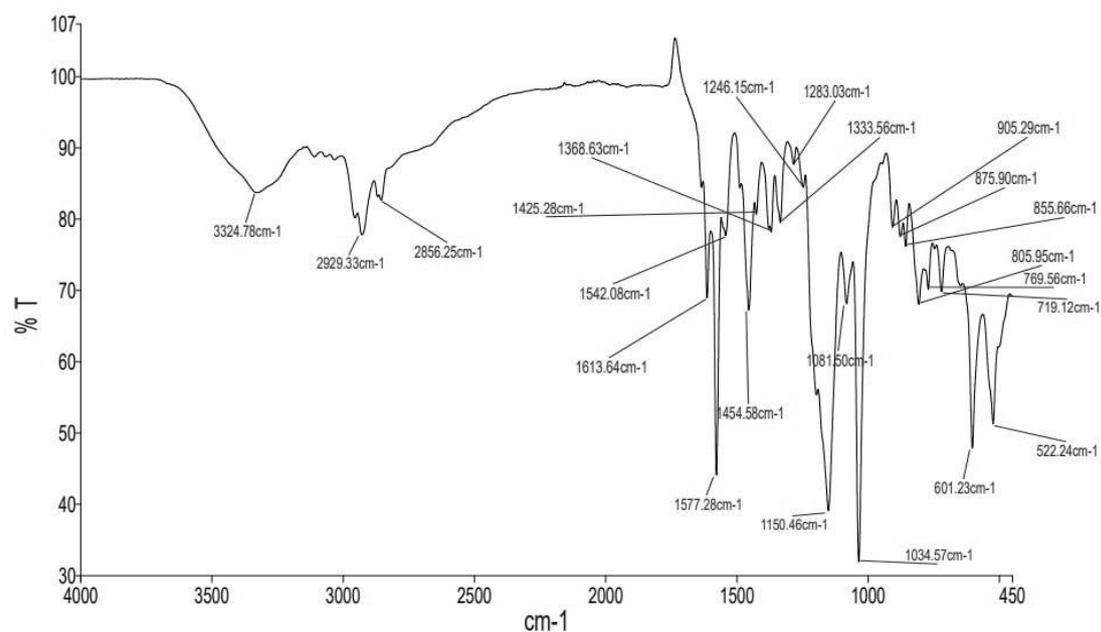


Figure S2. FTIR-ATR spectrum of [HCQH₂][C₆SO₃]₂.

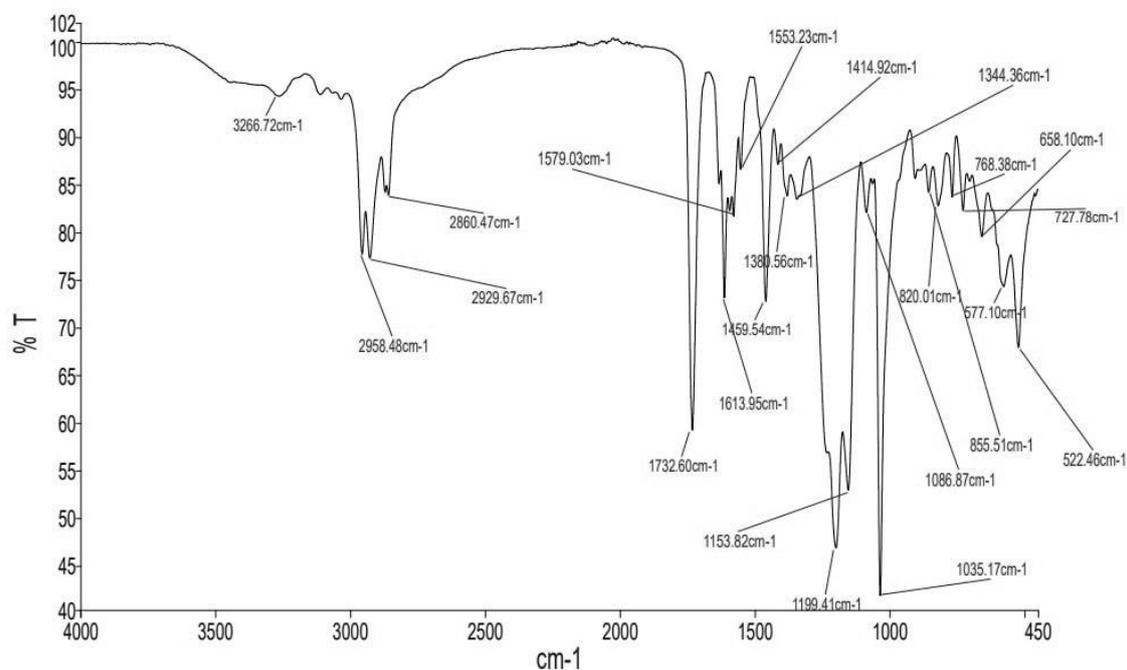


Figure S3. FTIR-ATR spectrum of [HCQH₂][DocSO₃]₂.

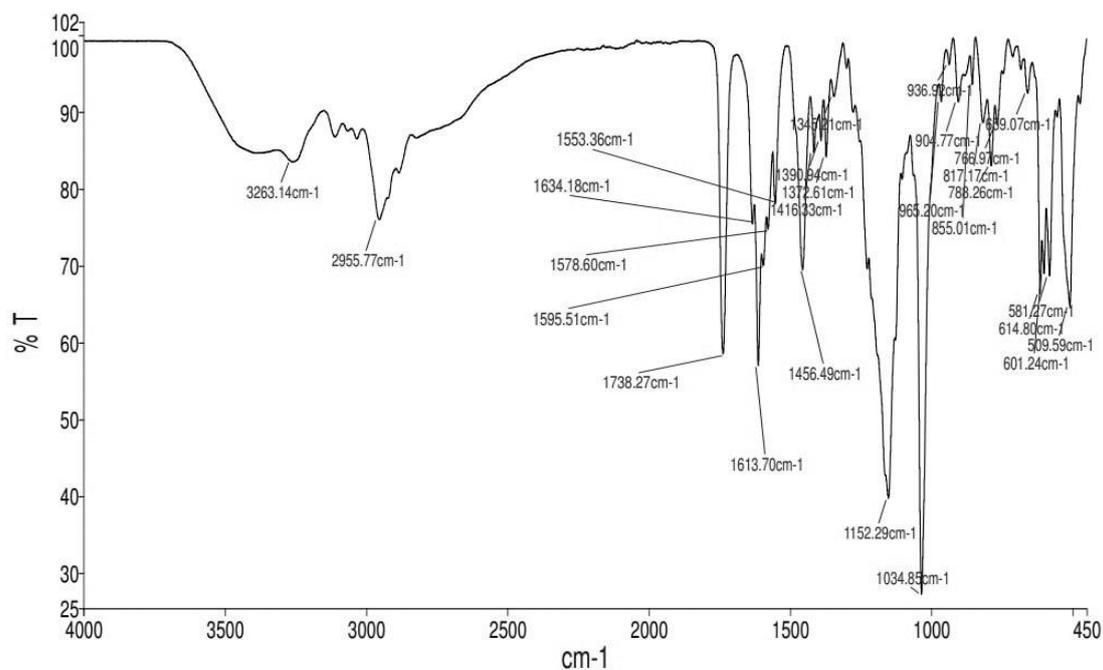


Figure S4. FTIR-ATR spectrum of [HCQH₂][CampSO₃]₂.

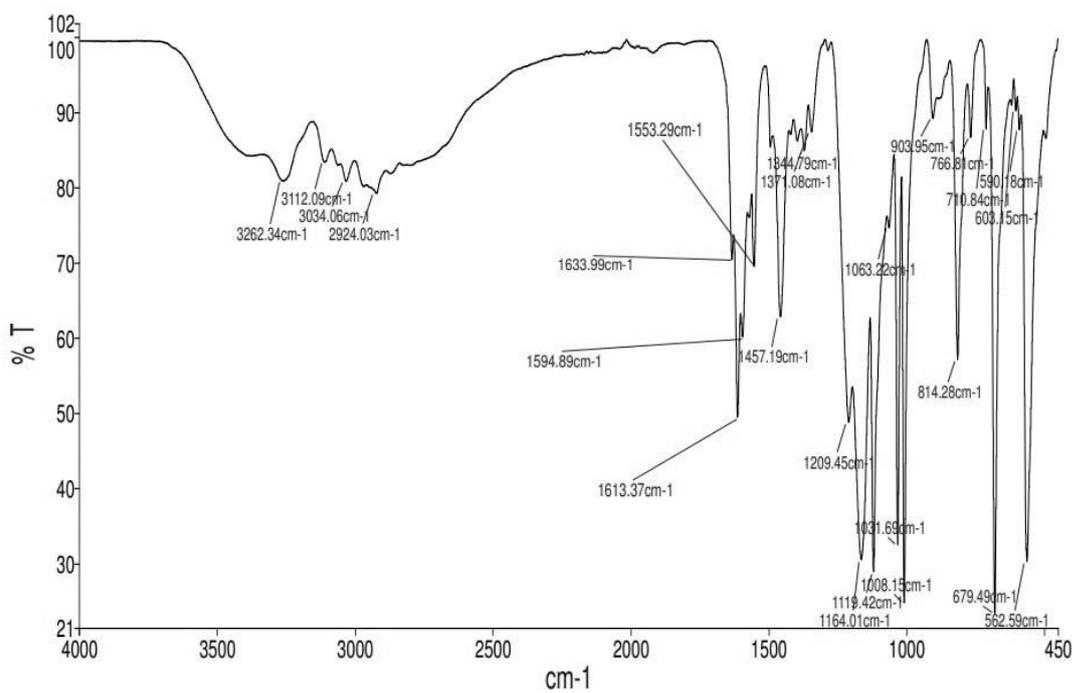


Figure S5. FTIR-ATR spectrum of $[\text{HCQH}_2][p\text{-TolSO}_3]_2$.

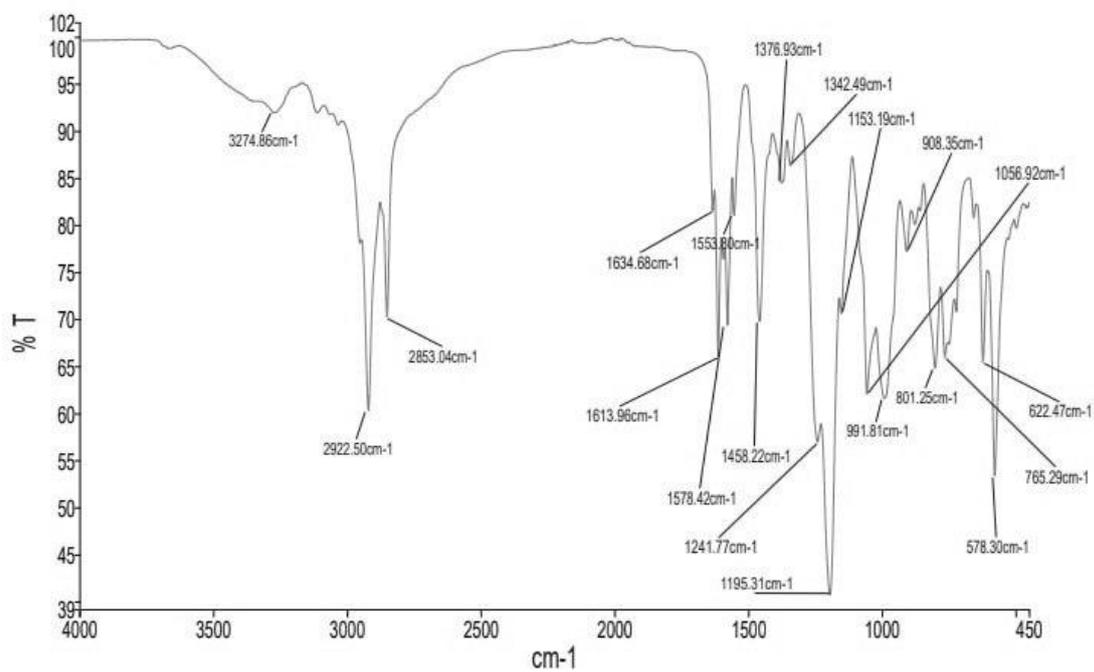


Figure S6. FTIR-ATR spectrum of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$.

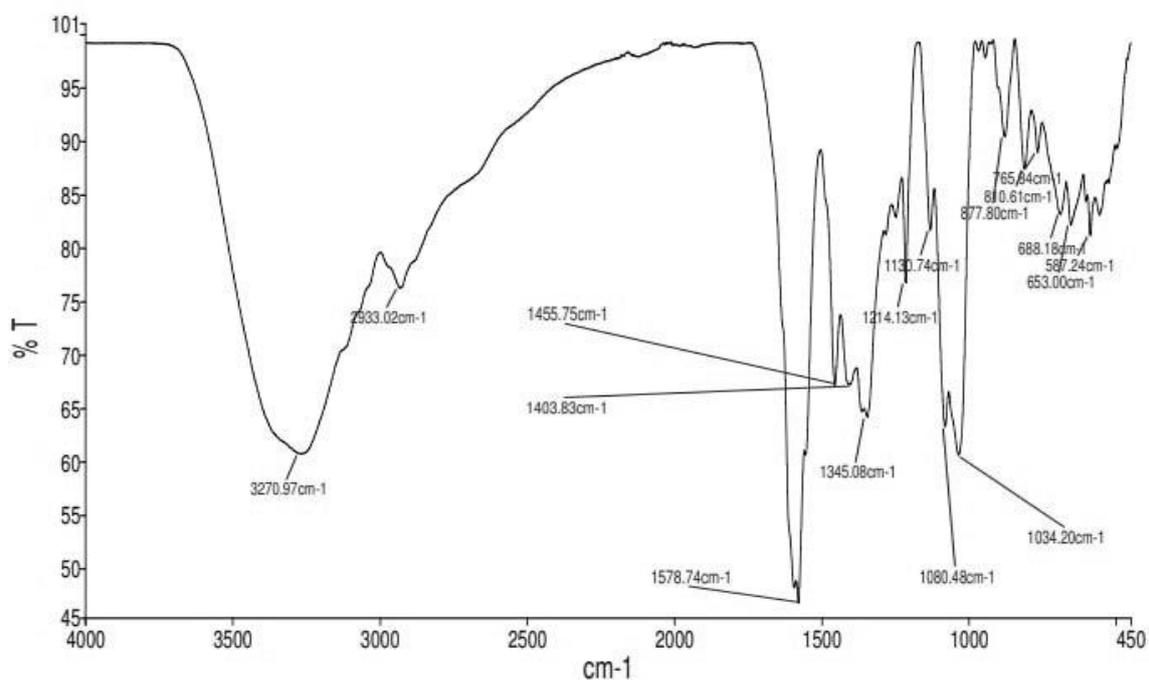


Figure S7. FTIR-ATR spectrum of [HCQH₂][GlcCOO]₂.

NMR spectra

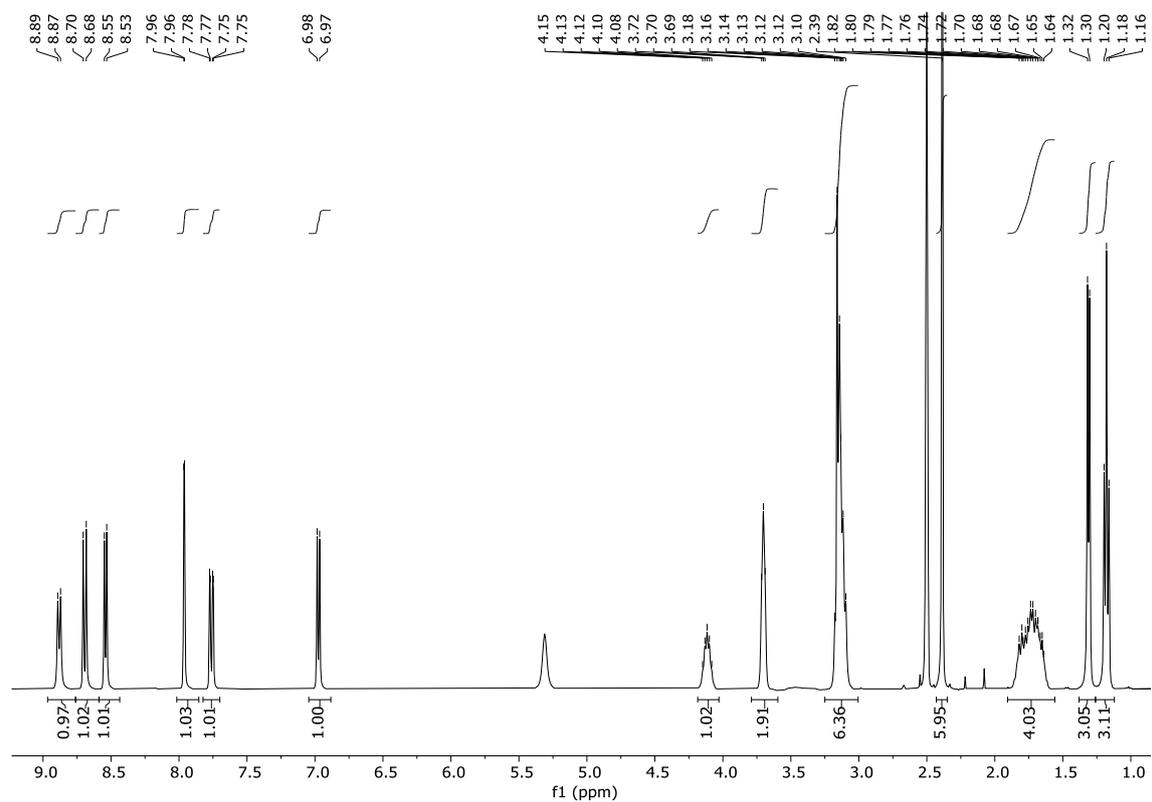


Figure S8. ^1H NMR spectrum of $[\text{HCQH}_2][\text{C}_1\text{SO}_3]_2$ in $\text{DMSO-}d_6$.

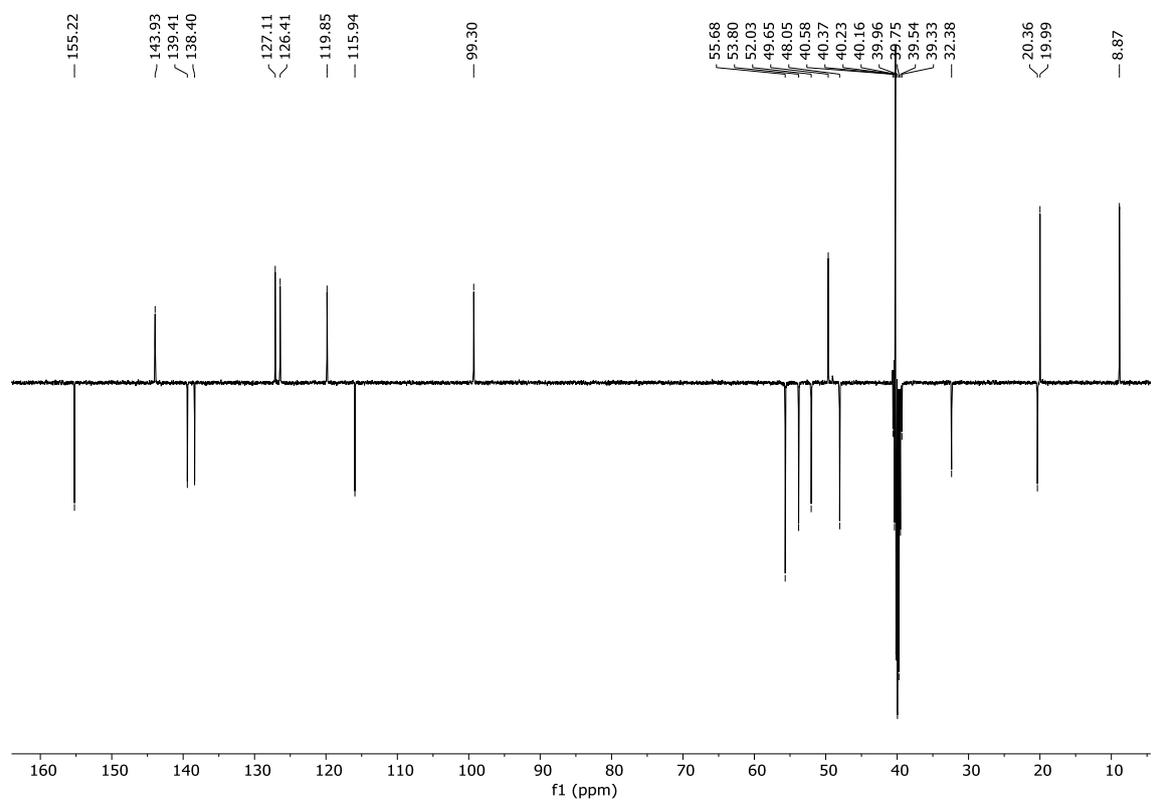


Figure S9. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][\text{C}_1\text{SO}_3]_2$ in $\text{DMSO-}d_6$.

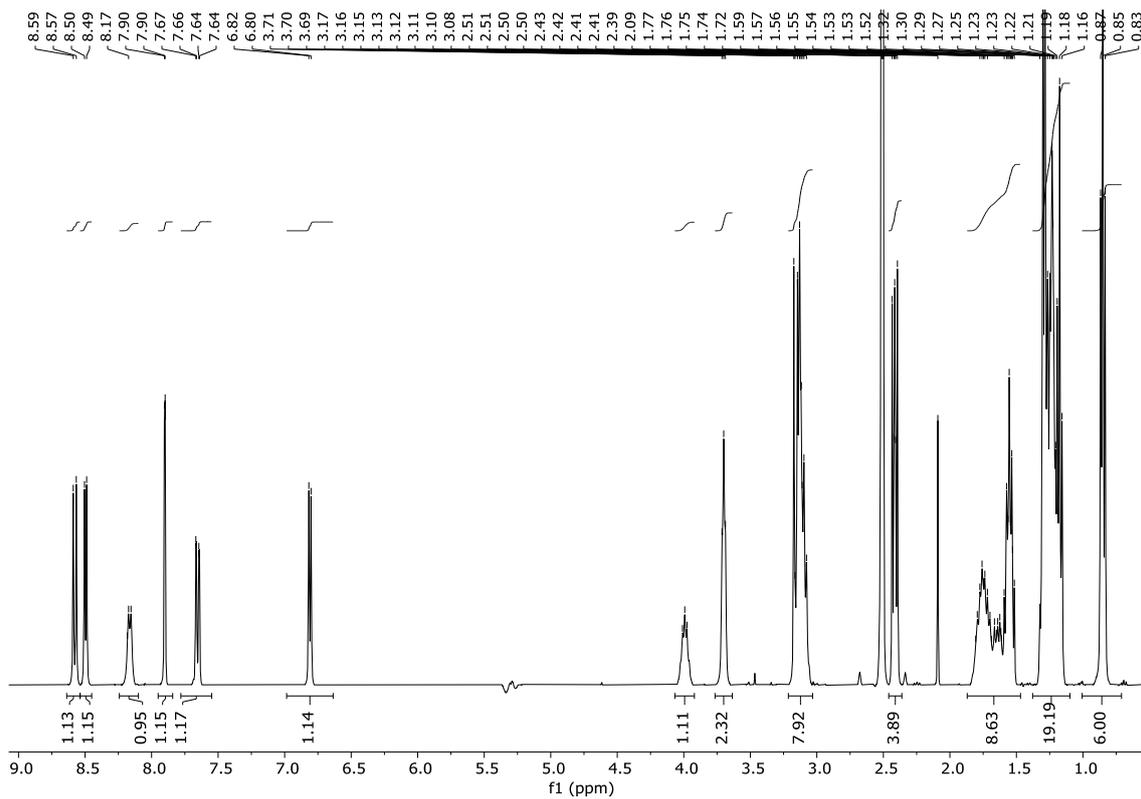


Figure S10. ^1H NMR spectrum of $[\text{HCQH}_2][\text{C}_6\text{SO}_3]_2$ in $\text{DMSO-}d_6$.

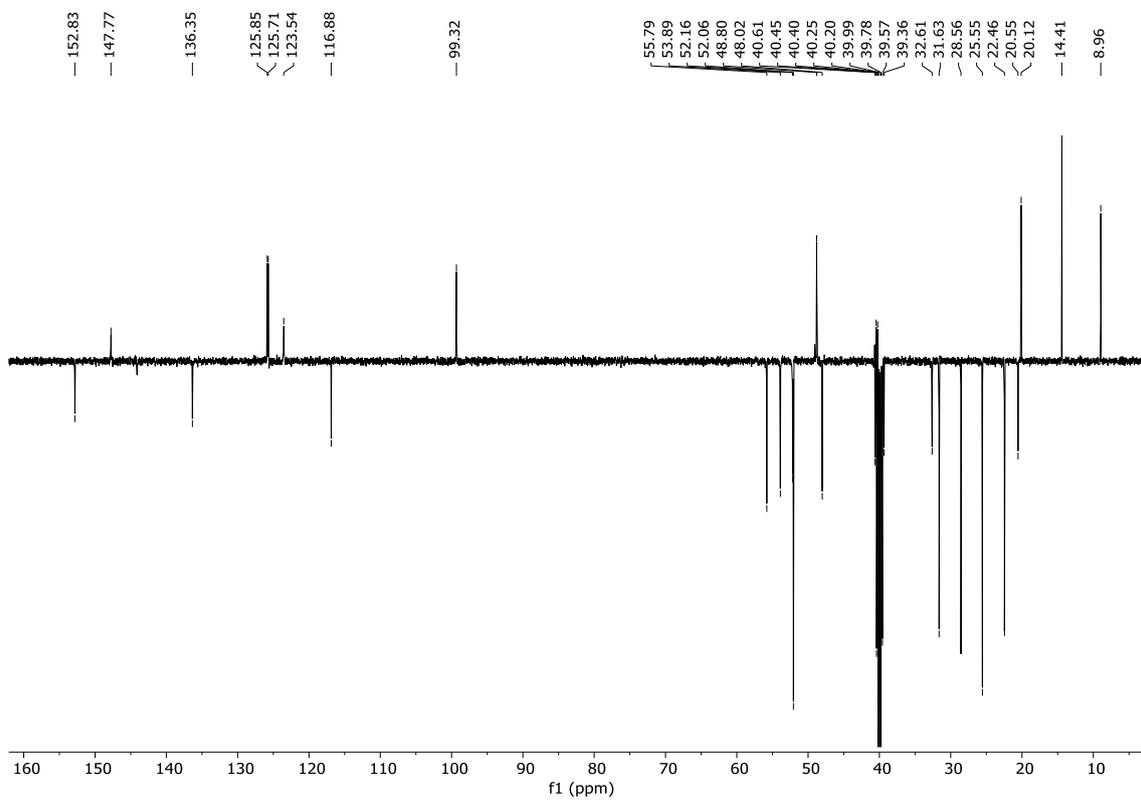


Figure S11. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][\text{C}_6\text{SO}_3]_2$ in $\text{DMSO-}d_6$.

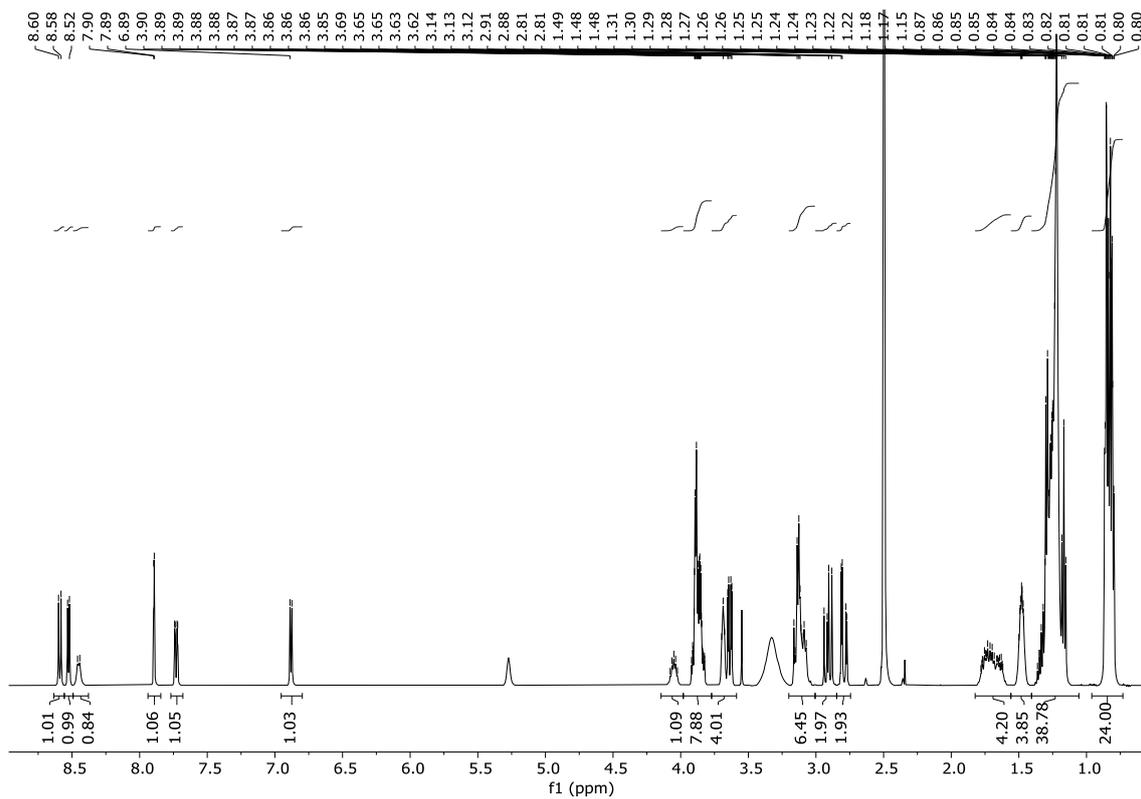


Figure S12. ^1H NMR spectrum of $[\text{HCQH}_2][\text{DocSO}_3]_2$ in $\text{DMSO-}d_6$.

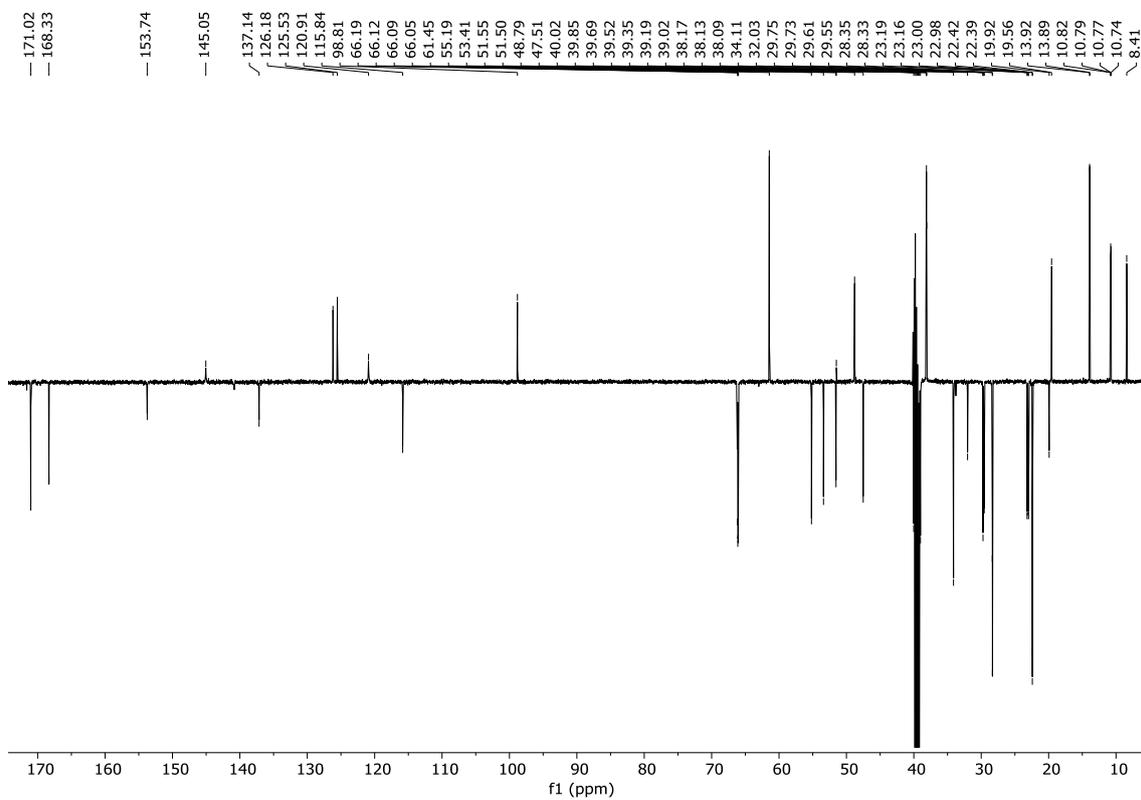


Figure S13. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][\text{DocSO}_3]_2$ in $\text{DMSO-}d_6$.

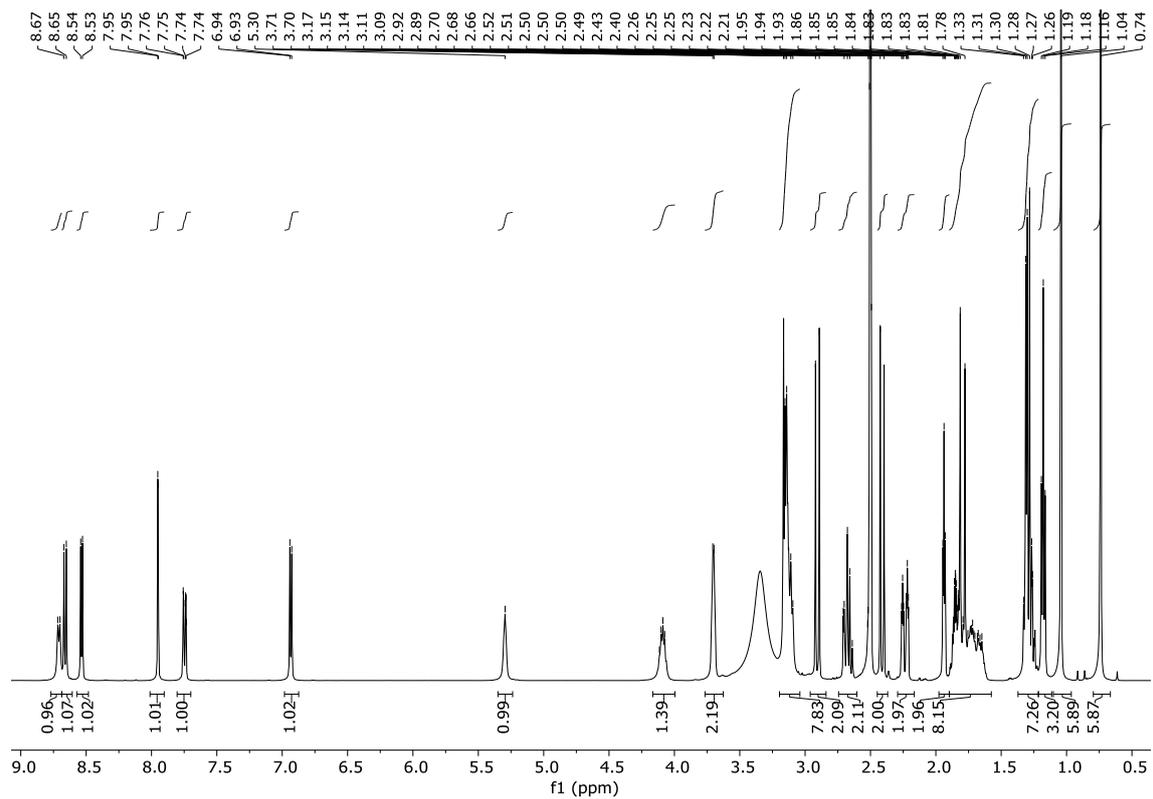


Figure S14. ^1H NMR spectrum of $[\text{HCQH}_2][\text{CampSO}_3]_2$ in $\text{DMSO-}d_6$.

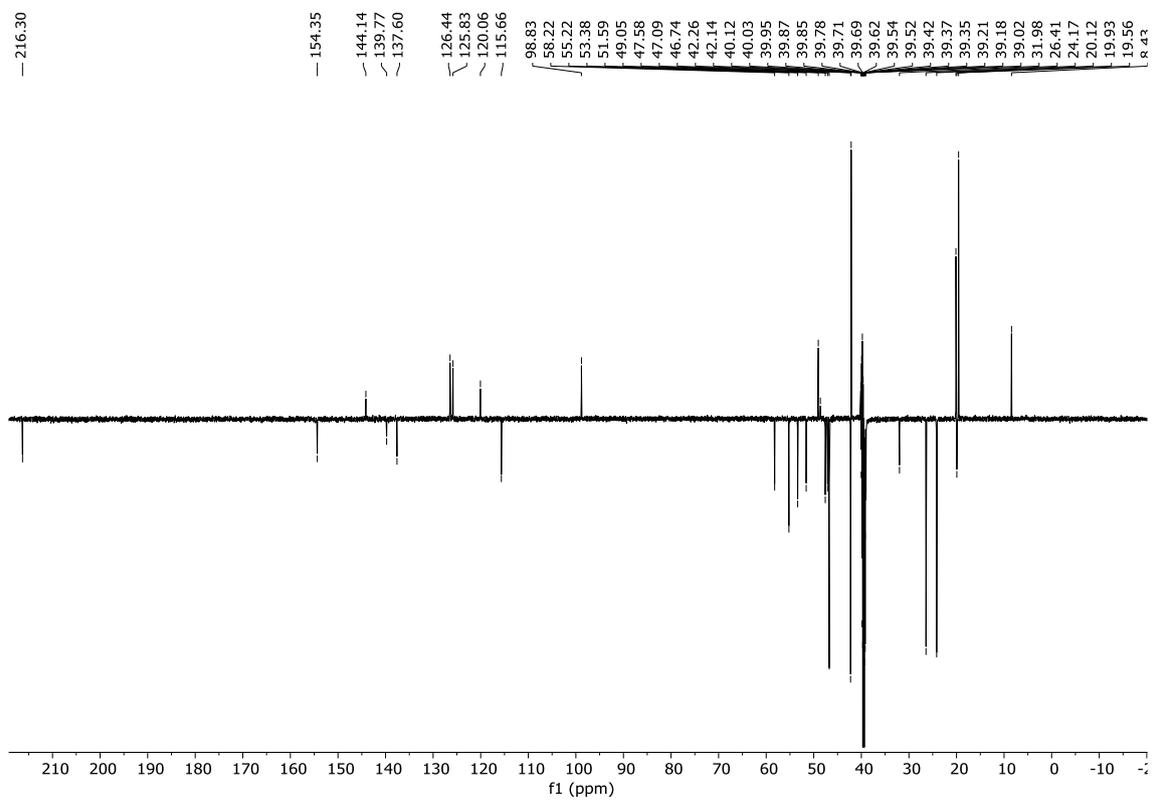


Figure S15. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][\text{CampSO}_3]_2$ in $\text{DMSO-}d_6$.

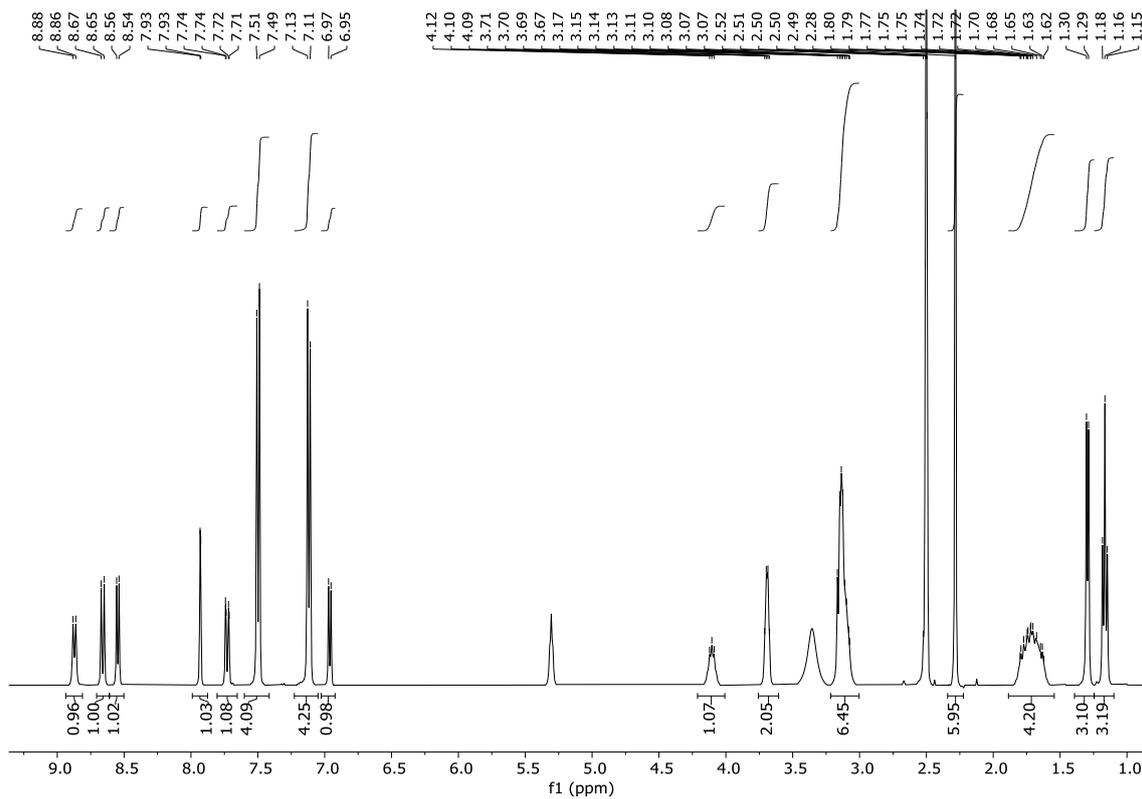


Figure S16. ^1H NMR spectrum of $[\text{HCQH}_2][p\text{-TolSO}_3]_2$ in $\text{DMSO-}d_6$.

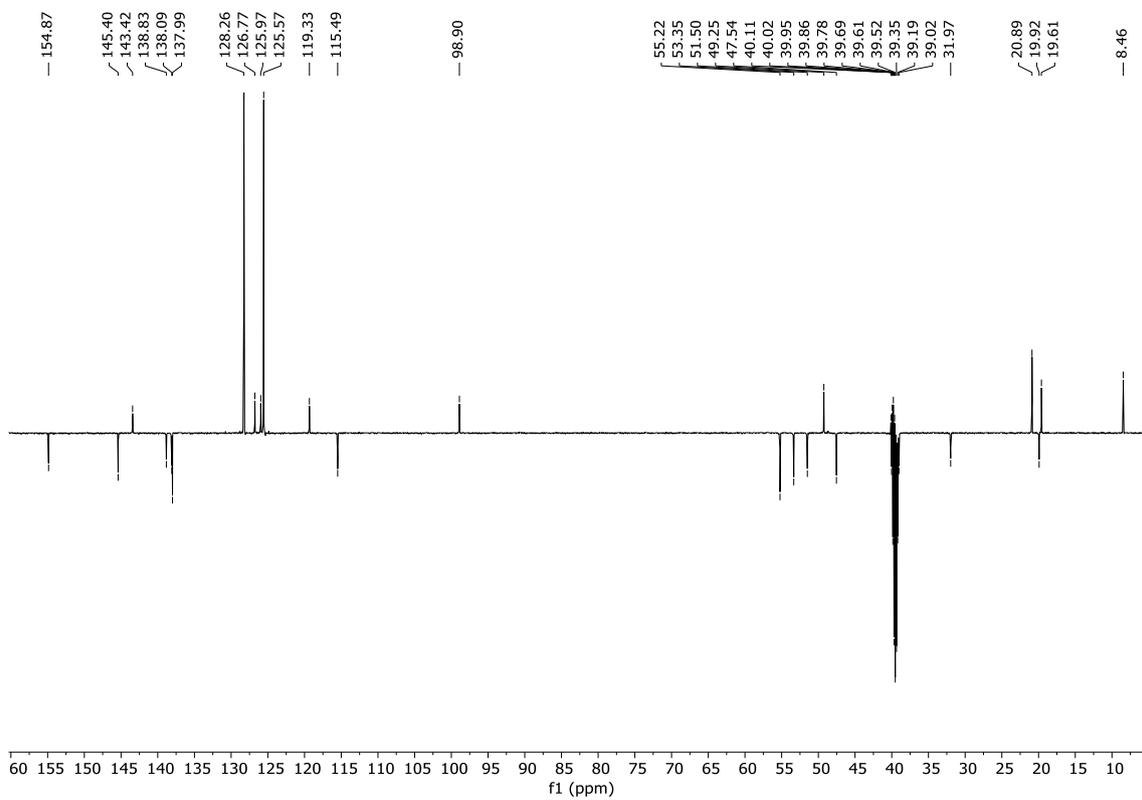


Figure S17. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][p\text{-TolSO}_3]_2$ in $\text{DMSO-}d_6$.

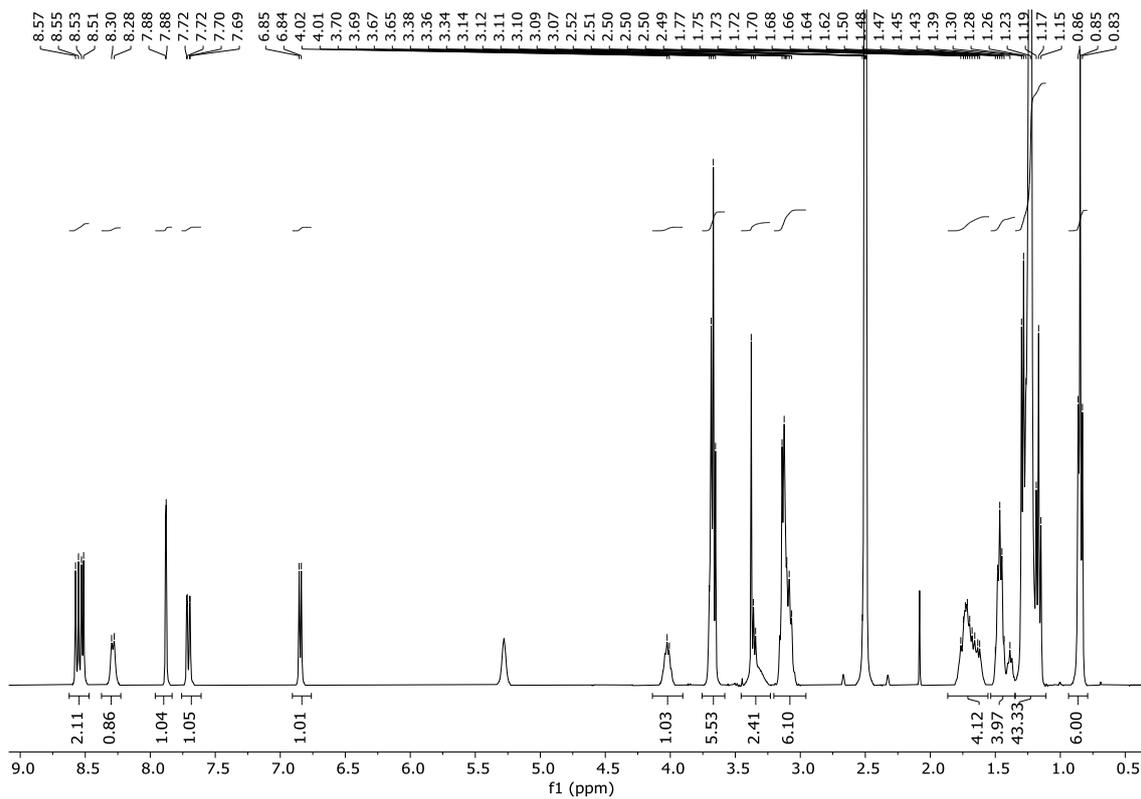


Figure S18. ^1H NMR spectrum of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$ in $\text{DMSO-}d_6$.

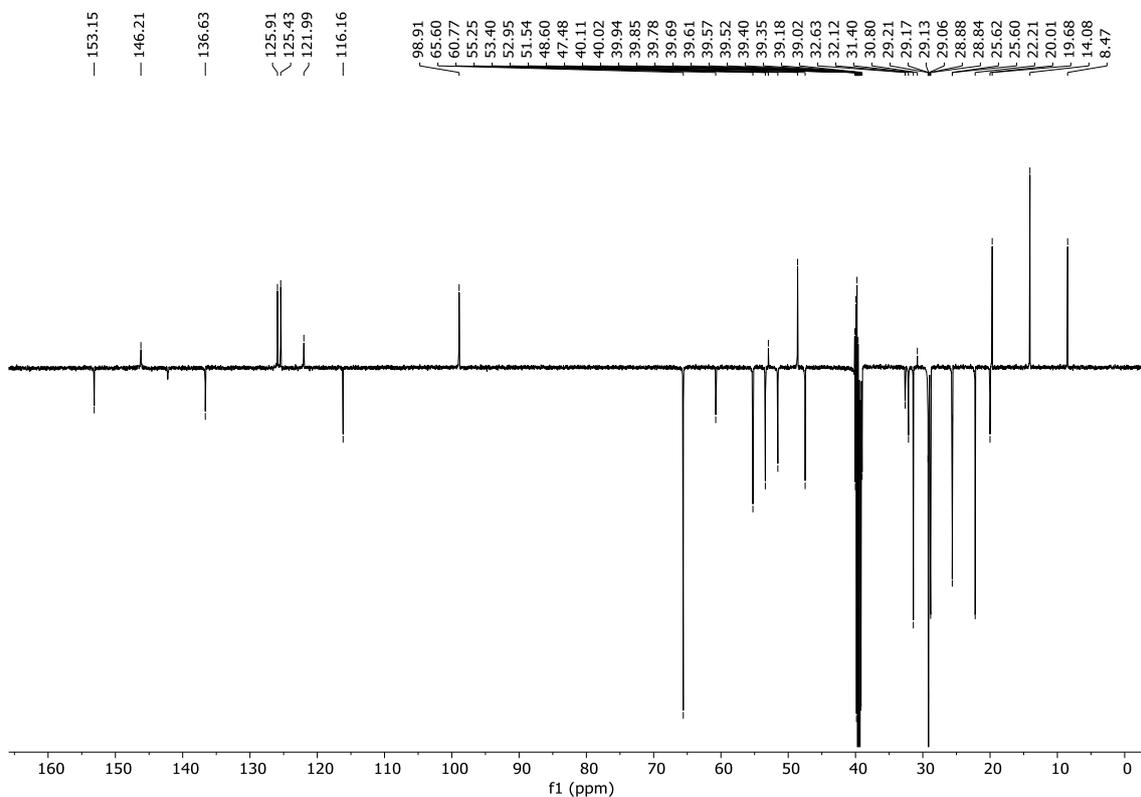


Figure S19. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$ in $\text{DMSO-}d_6$.

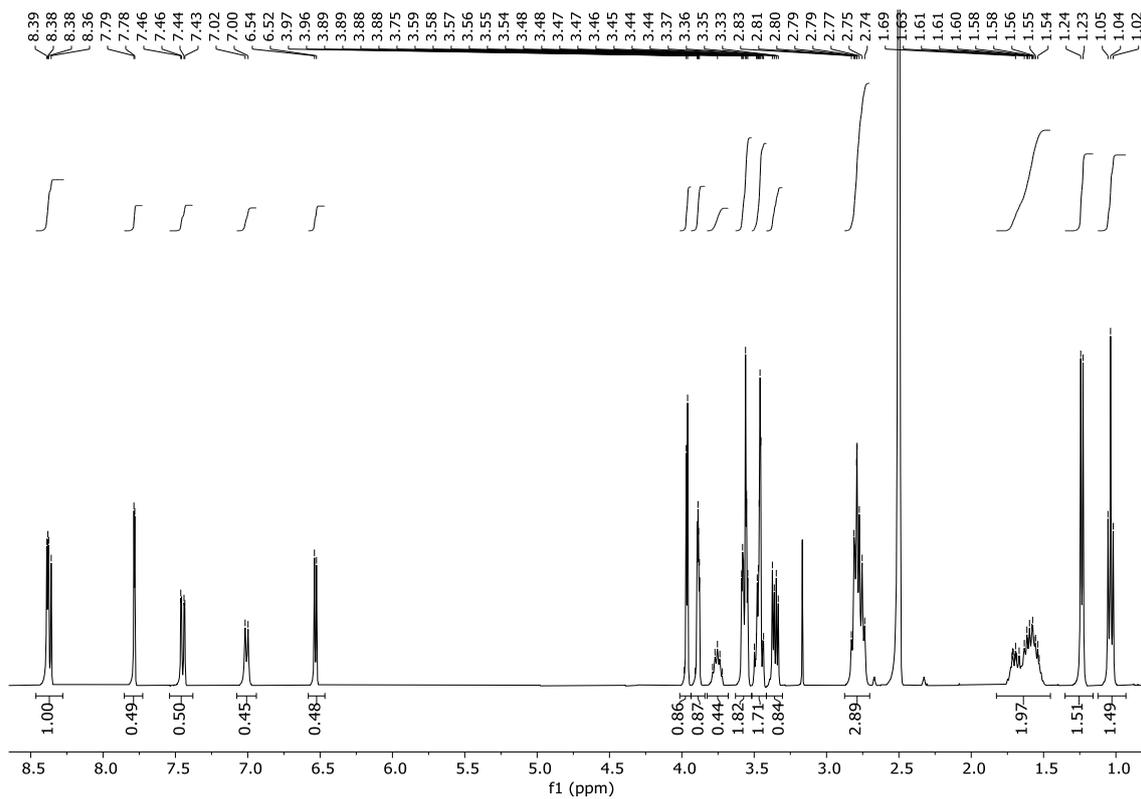


Figure S20. ^1H NMR spectrum of $[\text{HCQH}_2][\text{GlcCOO}]_2$ in $\text{DMSO-}d_6$.

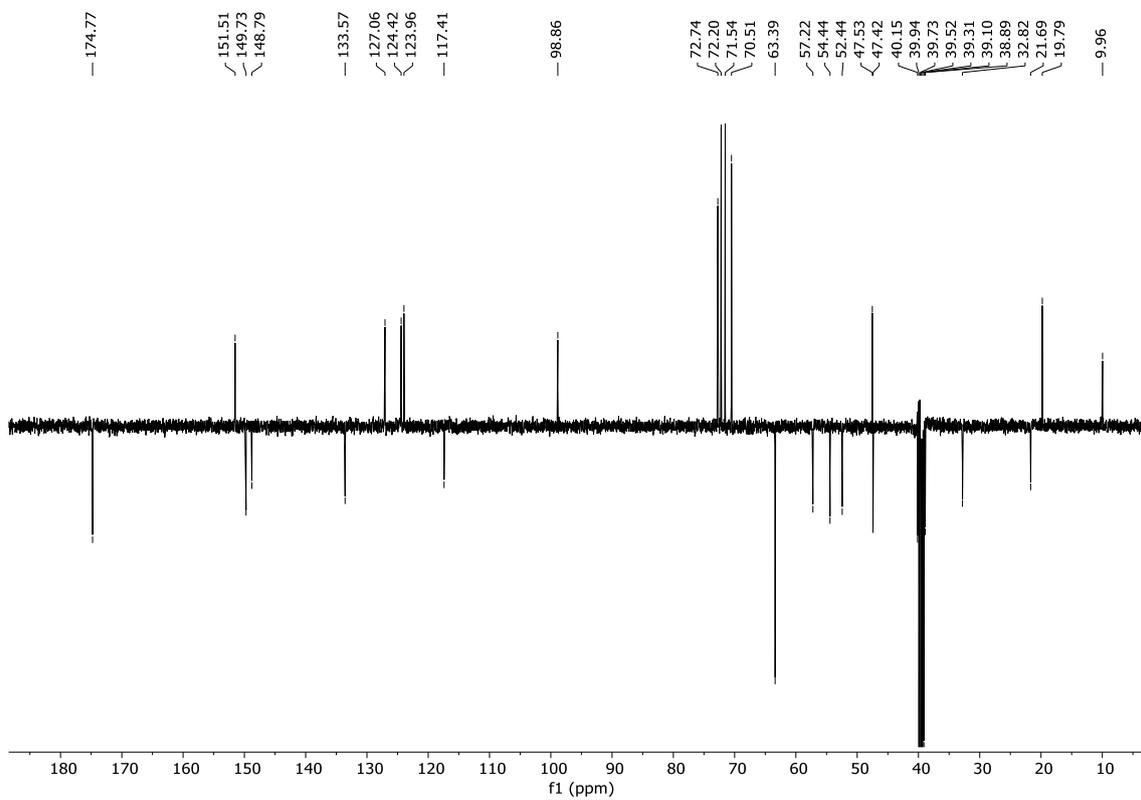


Figure S21. ^{13}C APT NMR spectrum of $[\text{HCQH}_2][\text{GlcCOO}]_2$ in $\text{DMSO-}d_6$.

HRMS spectra

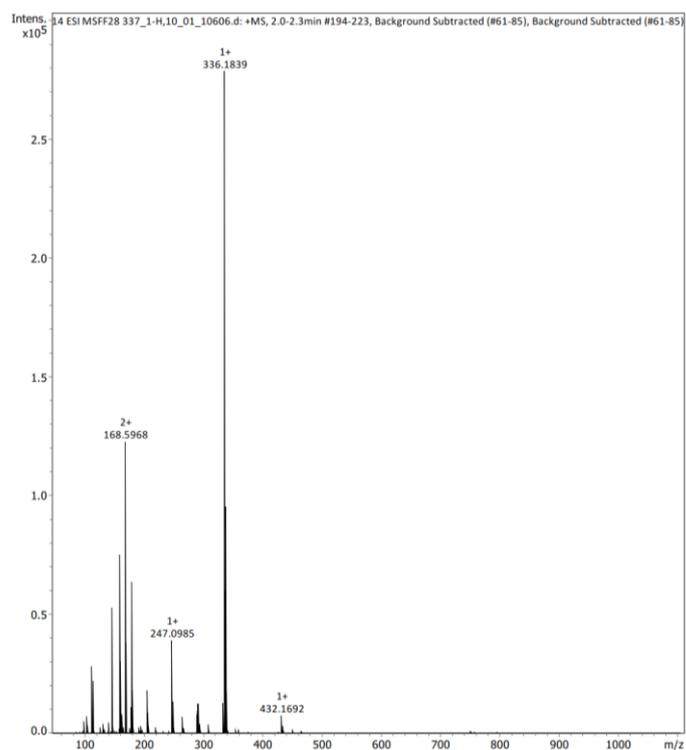


Figure S22. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][\text{C}_1\text{SO}_3]_2$.

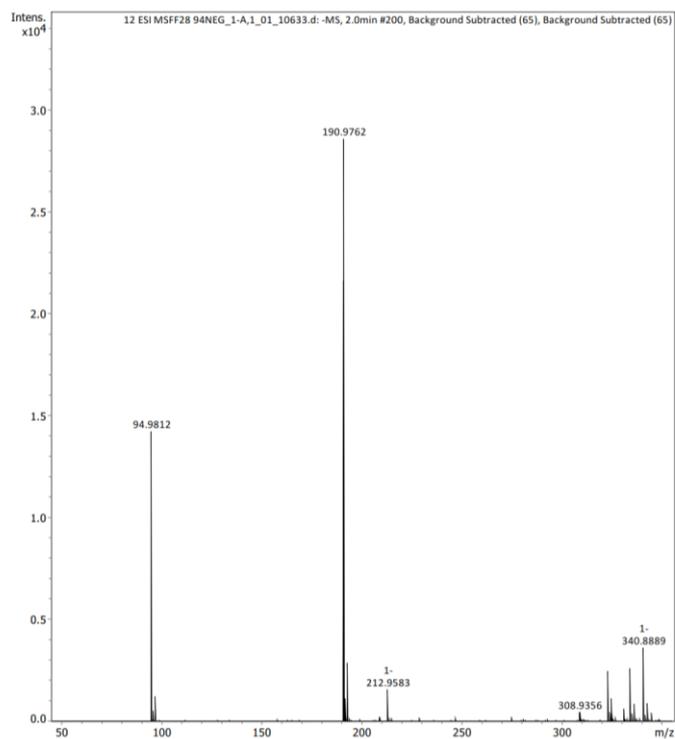


Figure S23. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][\text{C}_1\text{SO}_3]_2$.

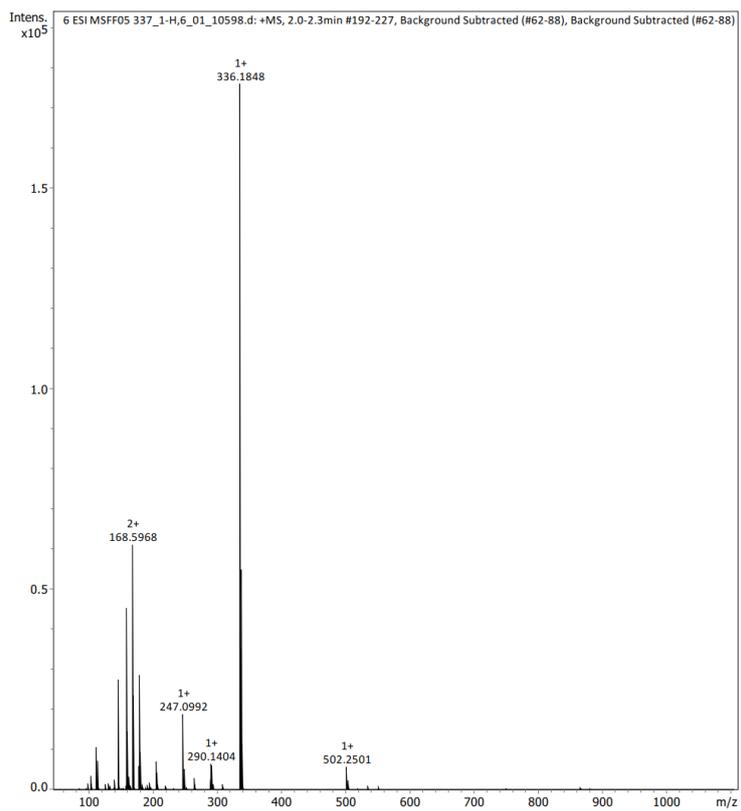


Figure S24. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][\text{C}_6\text{SO}_3]_2$.

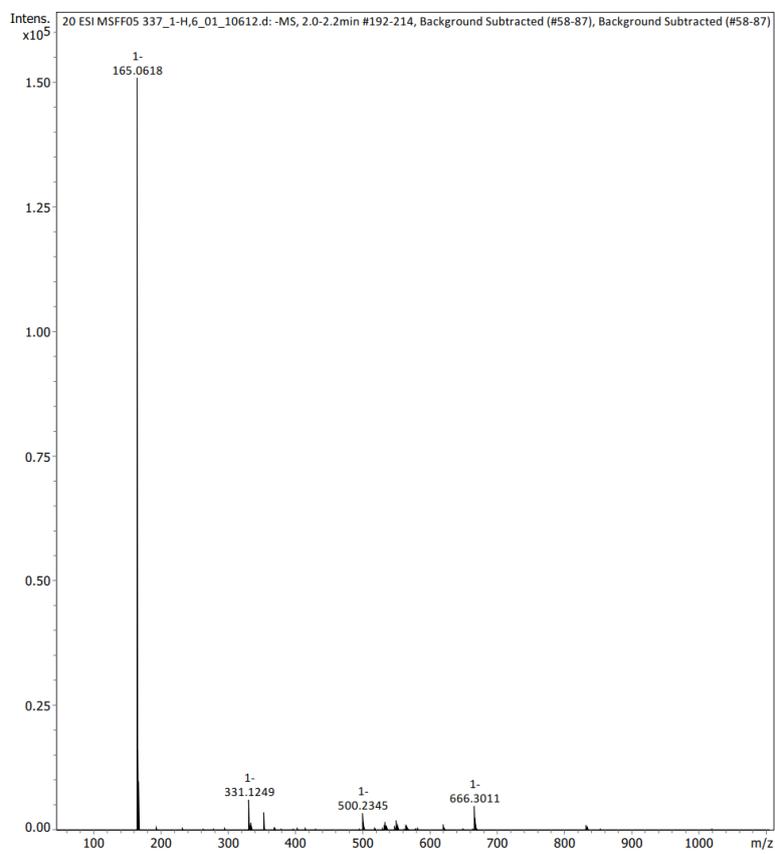


Figure S25. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][\text{C}_6\text{SO}_3]_2$.

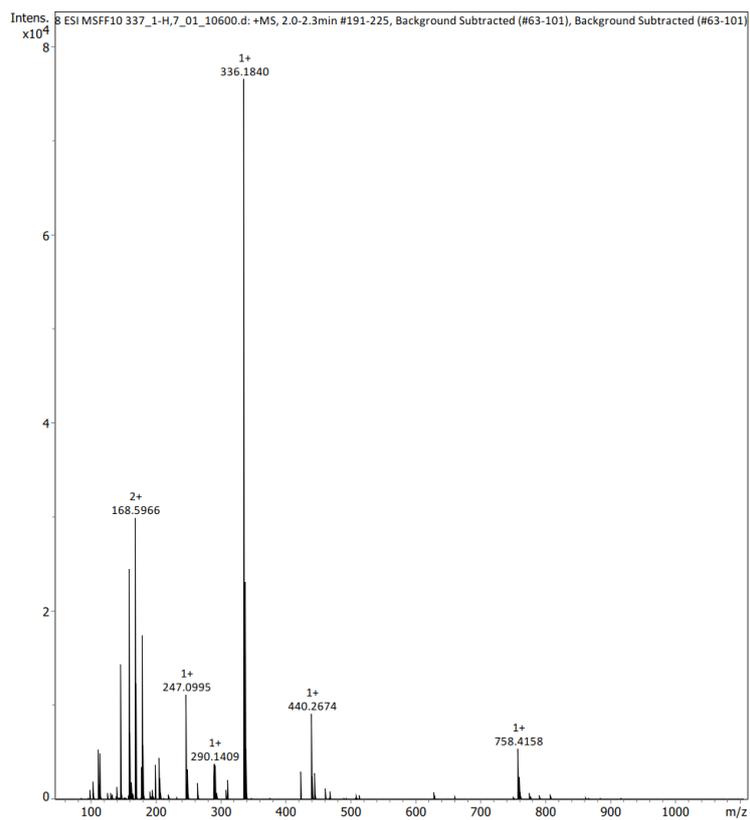


Figure S26. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][\text{DocSO}_3]_2$.

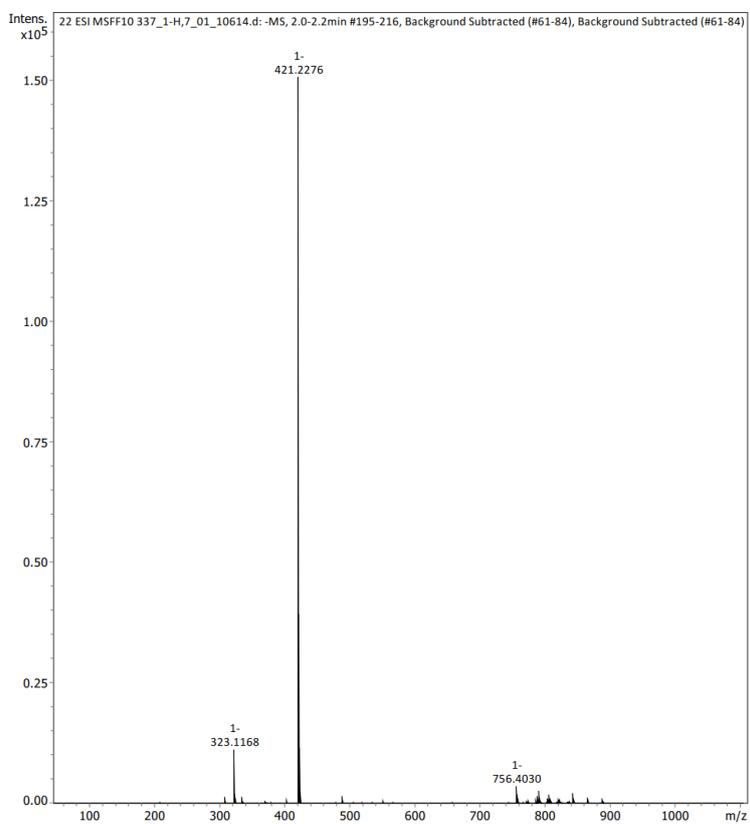


Figure S27. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][\text{DocSO}_3]_2$.

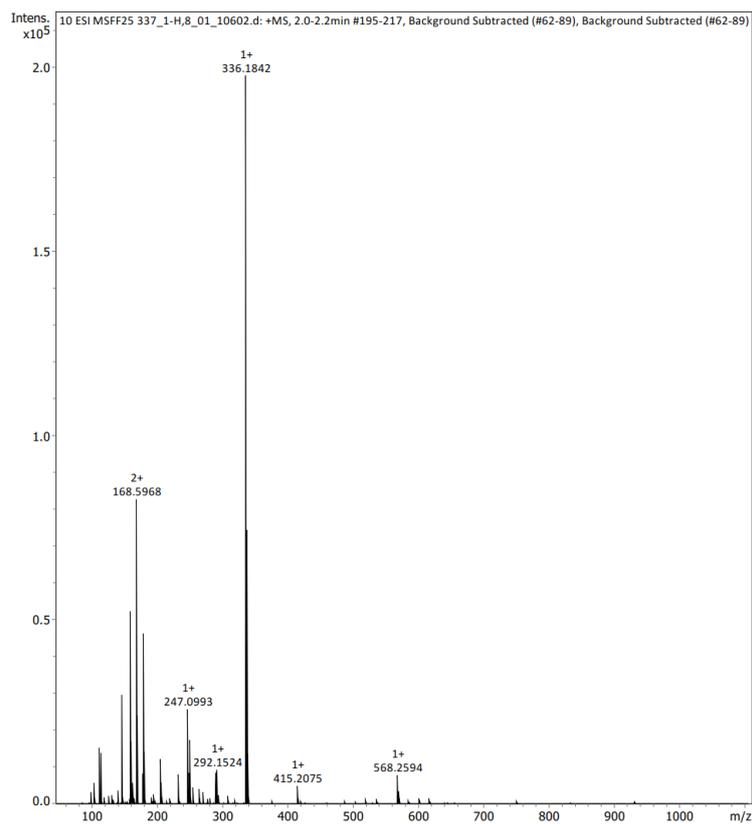


Figure S28. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][\text{CampSO}_3]_2$.

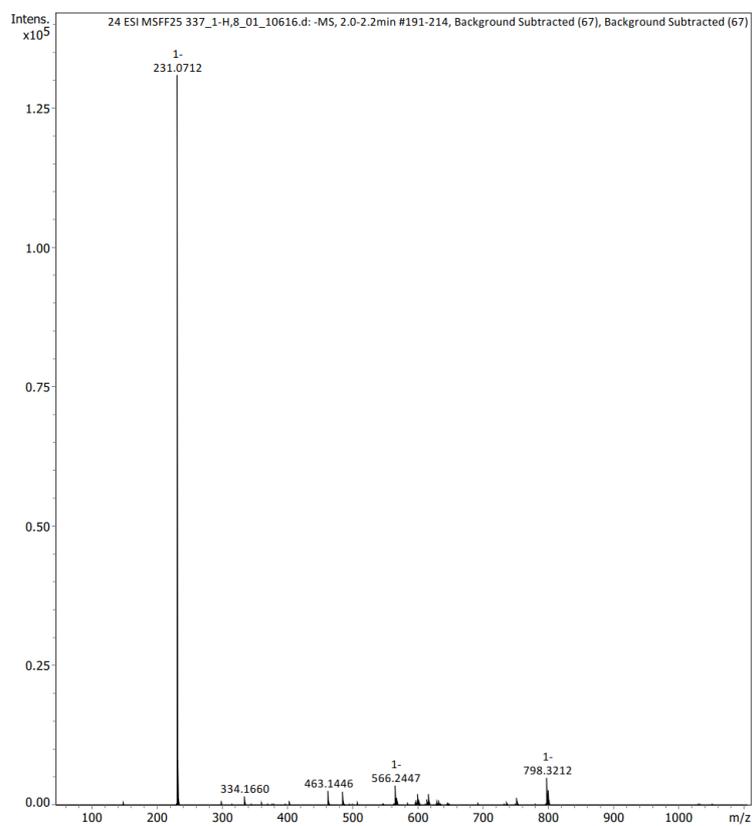


Figure S29. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][\text{CampSO}_3]_2$.

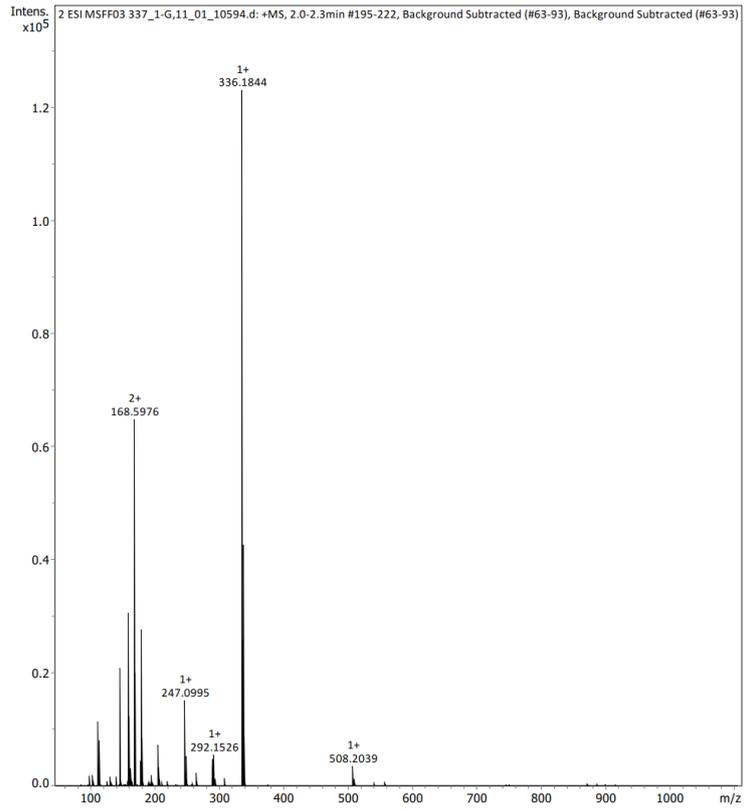


Figure S30. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][p\text{-TolSO}_3]_2$.

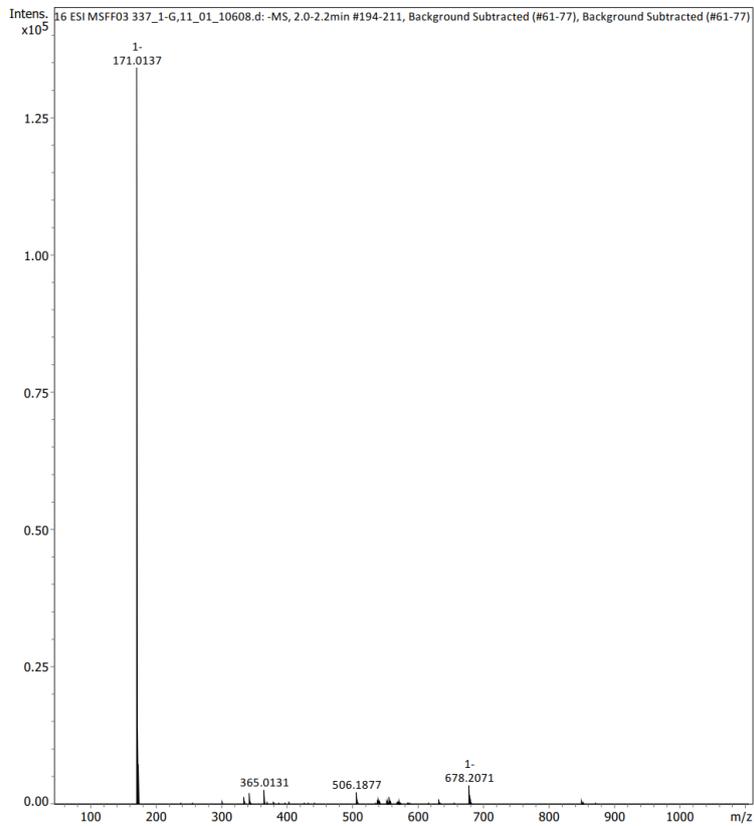


Figure S31. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][p\text{-TolSO}_3]_2$.

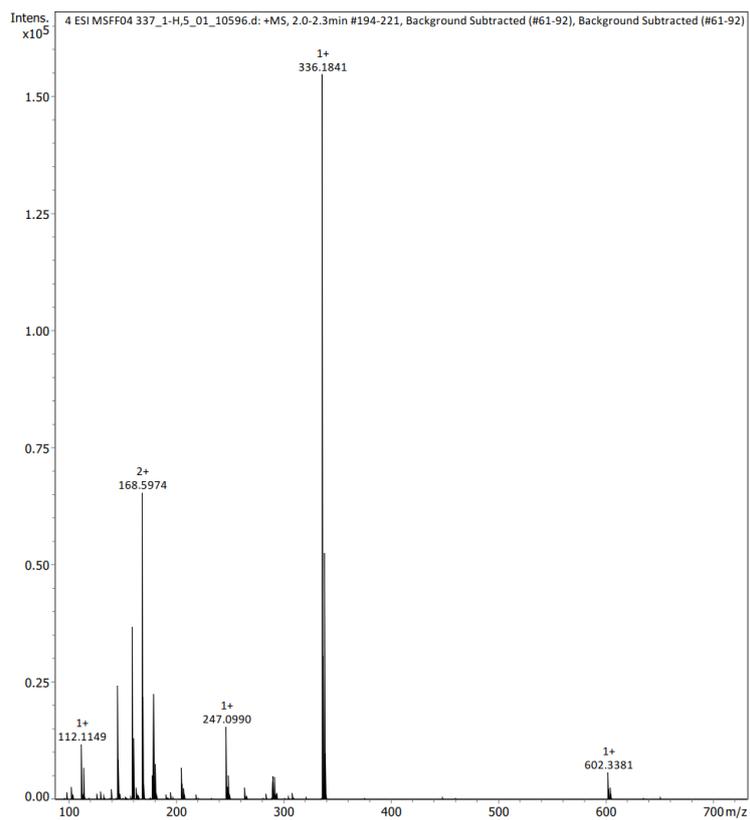


Figure S32. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$.

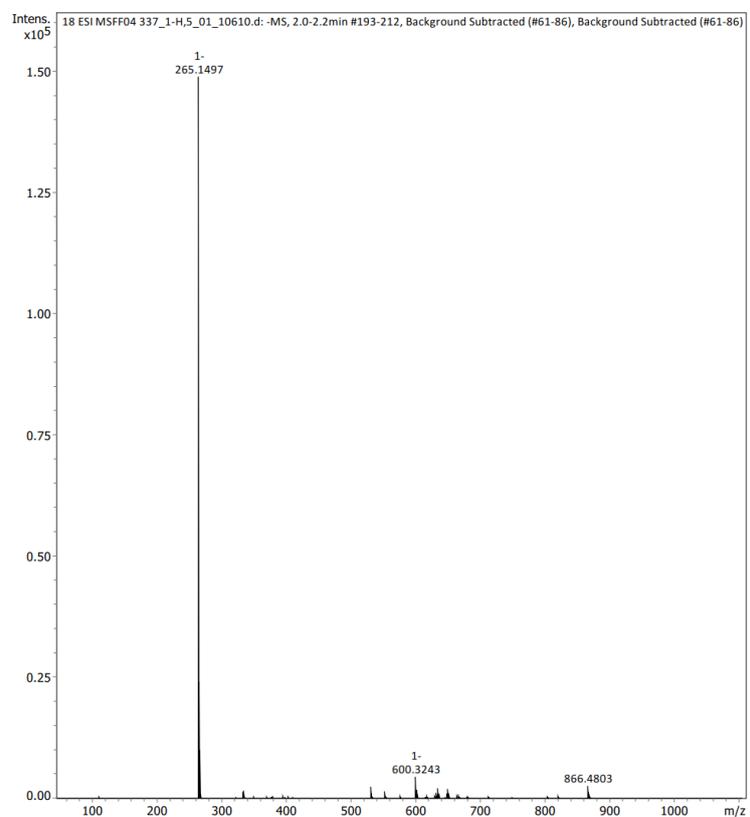


Figure S33. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$.

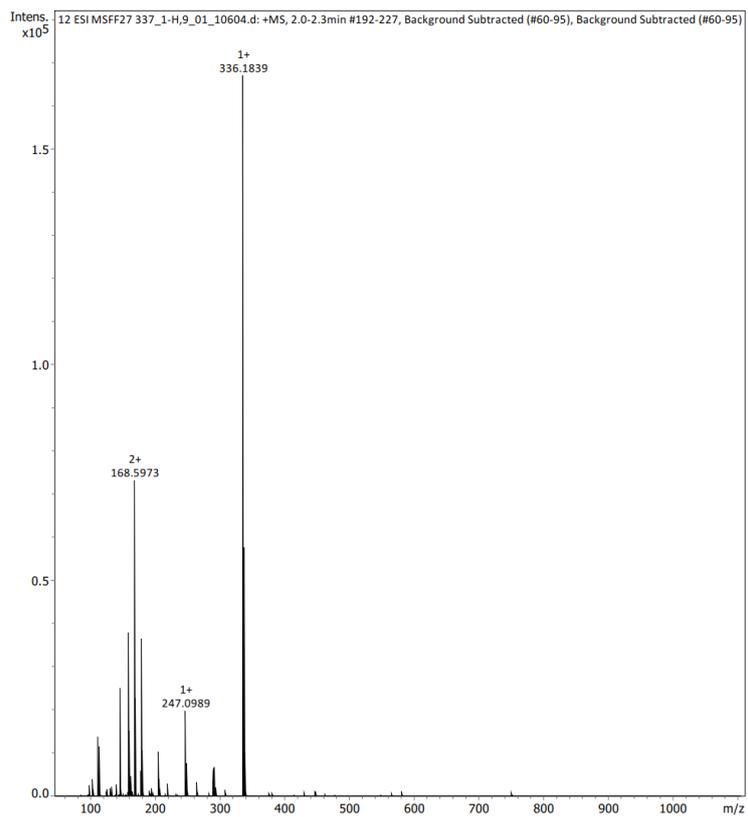


Figure S34. ESI-TOF mass spectra in positive mode of $[\text{HCQH}_2][\text{GlcCOO}]_2$.

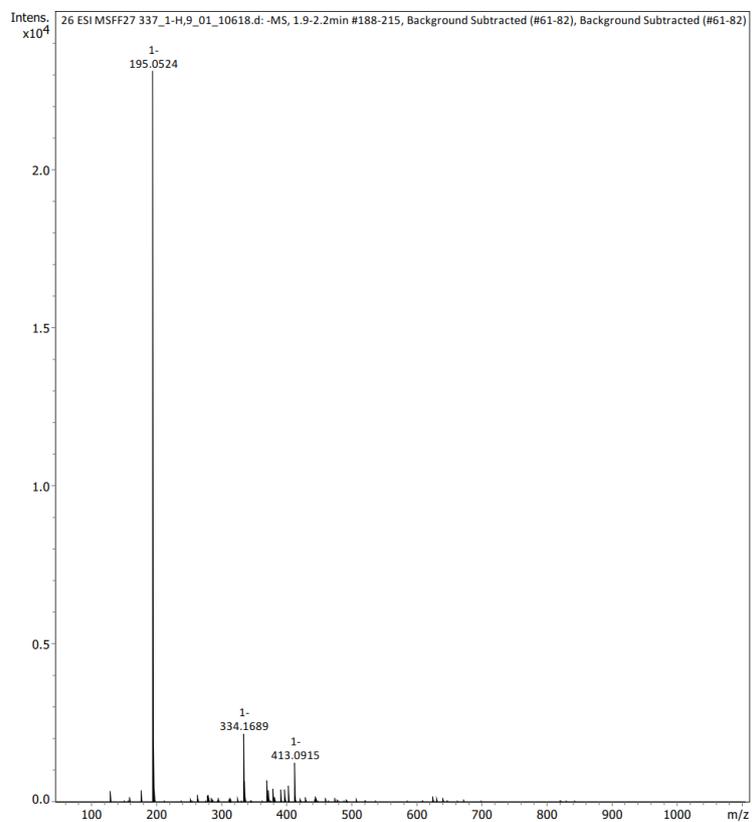


Figure S35. ESI-TOF mass spectra in negative mode of $[\text{HCQH}_2][\text{GlcCOO}]_2$.

Table S1. Experimental and calculated m/z values and corresponding errors (ppm) for the $[M+1]^+$ and $[M+2]^{2+}$ ions in positive mode of ESI-TOF for each HCQ-IL.

	Exp. m/z [M+1] ⁺	Calc. m/z [M+1] ⁺	error /ppm	Exp. m/z [M+2] ²⁺	Calc. m/z [M+2] ²⁺	error /ppm
[HCQH ₂][C ₁ SO ₃] ₂	336.1839	336.1837	-0.59	168.5968	168.5955	-7.71
[HCQH ₂][C ₆ SO ₃] ₂	336.1848	336.1837	-3.27	168.5968	168.5955	-7.71
[HCQH ₂][DocSO ₃] ₂	336.1840	336.1837	-0.89	168.5966	168.5955	-6.52
[HCQH ₂][CampSO ₃] ₂	336.1842	336.1837	-1.49	168.5968	168.5955	-7.71
[HCQH ₂][<i>p</i> -TolSO ₃] ₂	336.1844	336.1837	-2.08	168.5976	168.5955	-12.46
[HCQH ₂][C ₁₂ SO ₄] ₂	336.1841	336.1837	-1.19	168.5974	168.5955	-11.27
[HCQH ₂][GlcCOO] ₂	336.1839	336.1837	-0.59	168.5973	168.5955	-10.68

Table S2. Experimental and calculated m/z values and corresponding errors (ppm) for the $[M-1]^-$ ion in negative mode of ESI-TOF for each HCQ-IL.

	Exp. m/z [M-1] ⁻	Calc. m/z [M-1] ⁻	error /ppm
[HCQH ₂][C ₁ SO ₃] ₂	94.9808	94.9812	4.21
[HCQH ₂][C ₆ SO ₃] ₂	165.0618	165.0590	-16.96
[HCQH ₂][DocSO ₃] ₂	421.2276	421.2265	-2.61
[HCQH ₂][CampSO ₃] ₂	231.0696	231.0712	6.92
[HCQH ₂][<i>p</i> -TolSO ₃] ₂	171.0137	171.0121	-9.36
[HCQH ₂][C ₁₂ SO ₄] ₂	265.1497	265.1479	-6.79
[HCQH ₂][GlcCOO] ₂	195.0510	195.0524	7.18

DSC thermograms

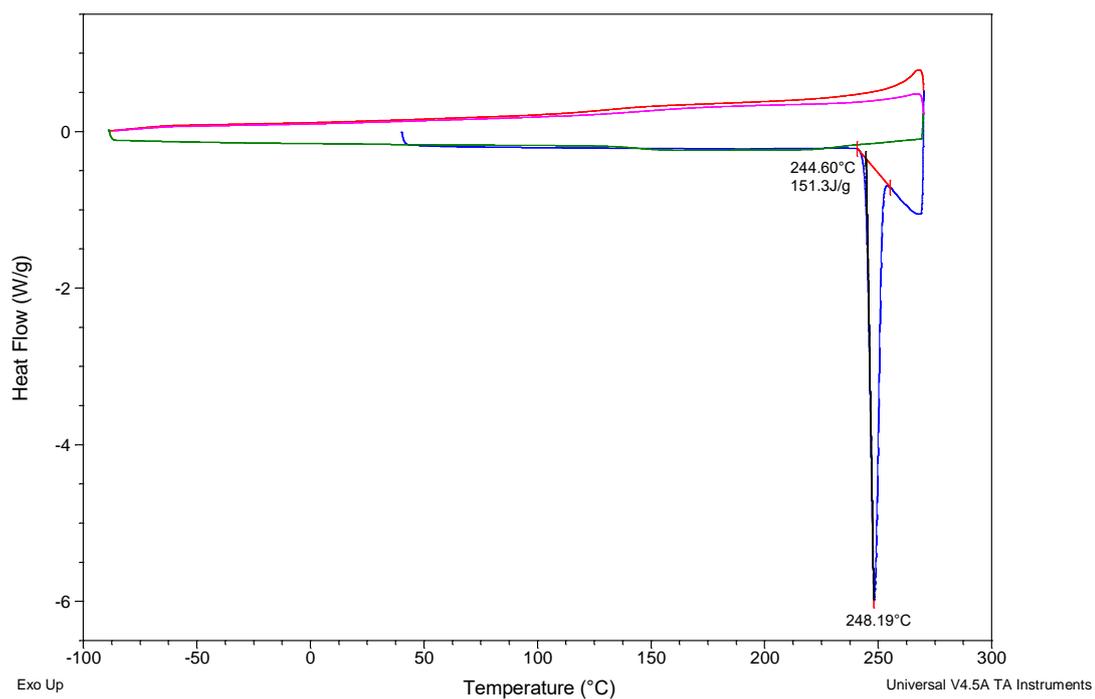


Figure S36. DSC thermogram of [HCQH₂][SO₄].

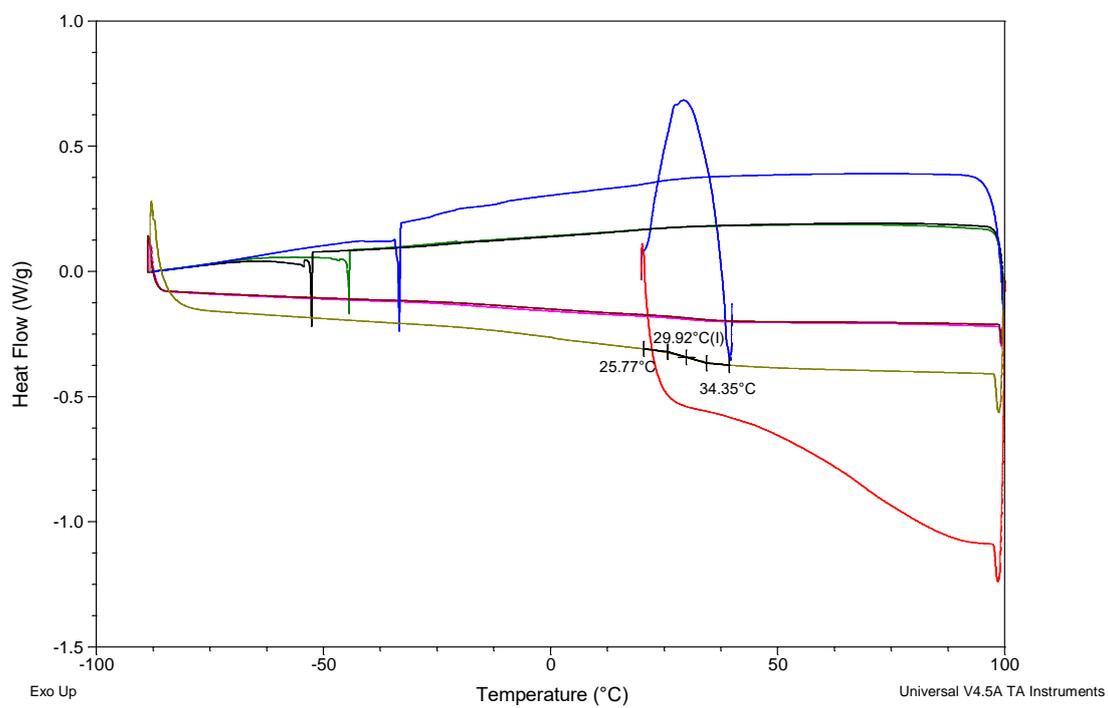


Figure S37. DSC thermogram of [HCQH₂][C₁SO₃]₂.

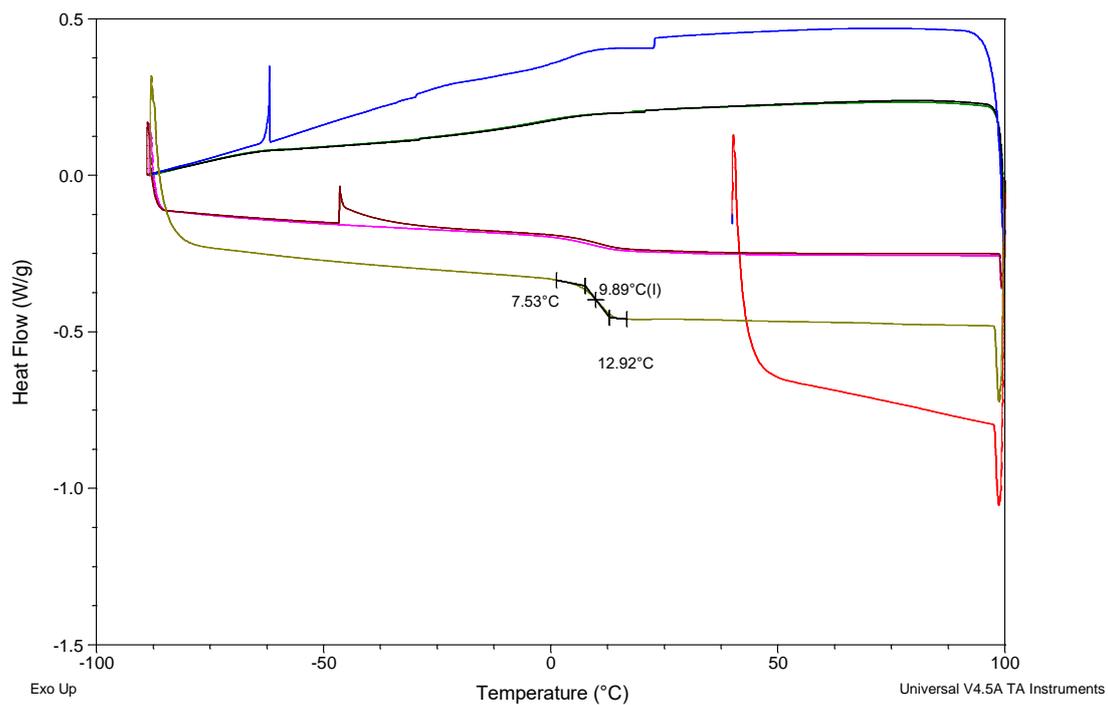


Figure S38. DSC thermogram of [HCQH₂][C₆SO₃]₂.

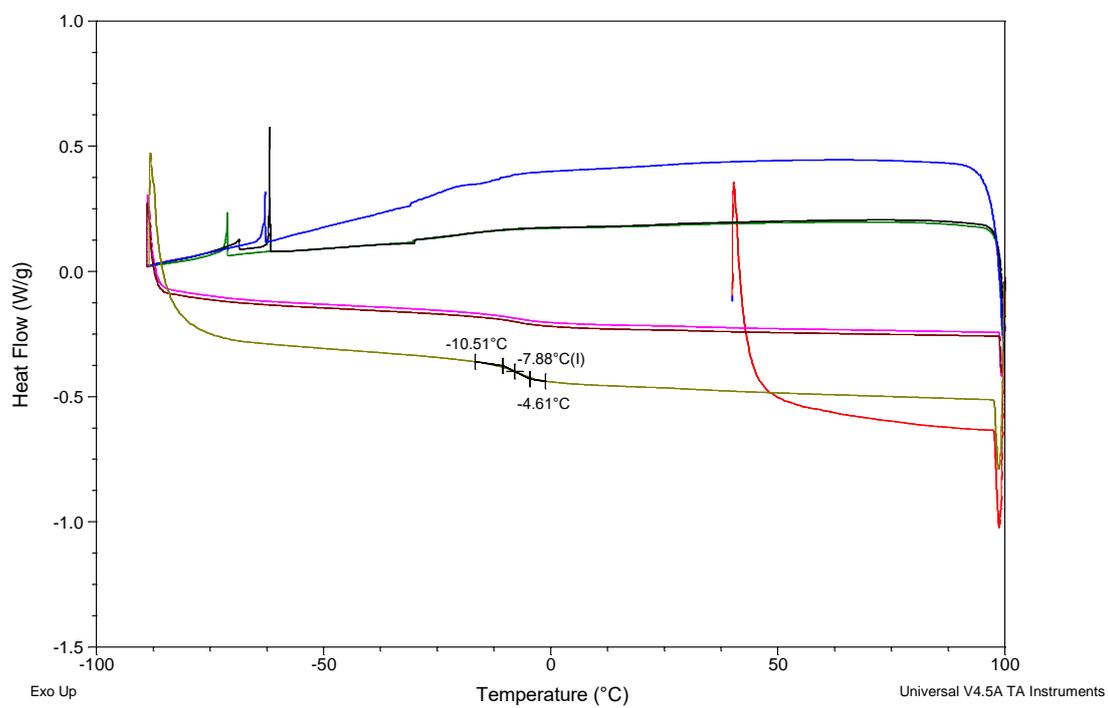


Figure S39. DSC thermogram of [HCQH₂][DocSO₃]₂.

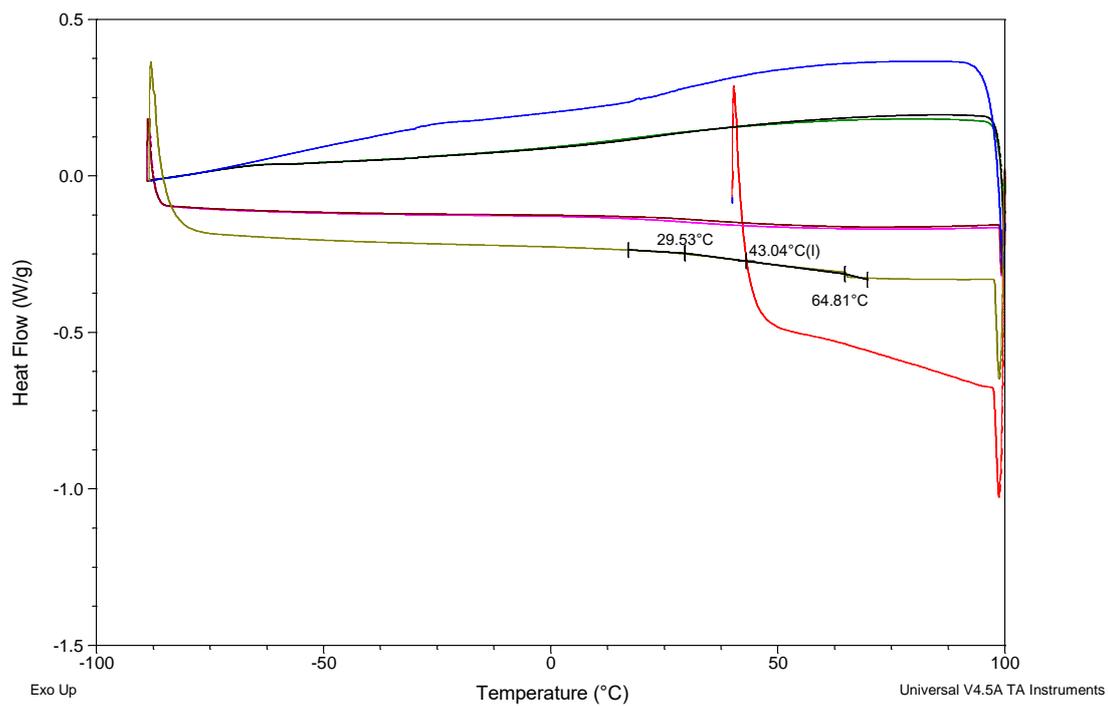


Figure S40. DSC thermogram of [HCQH₂][CampSO₃]₂.

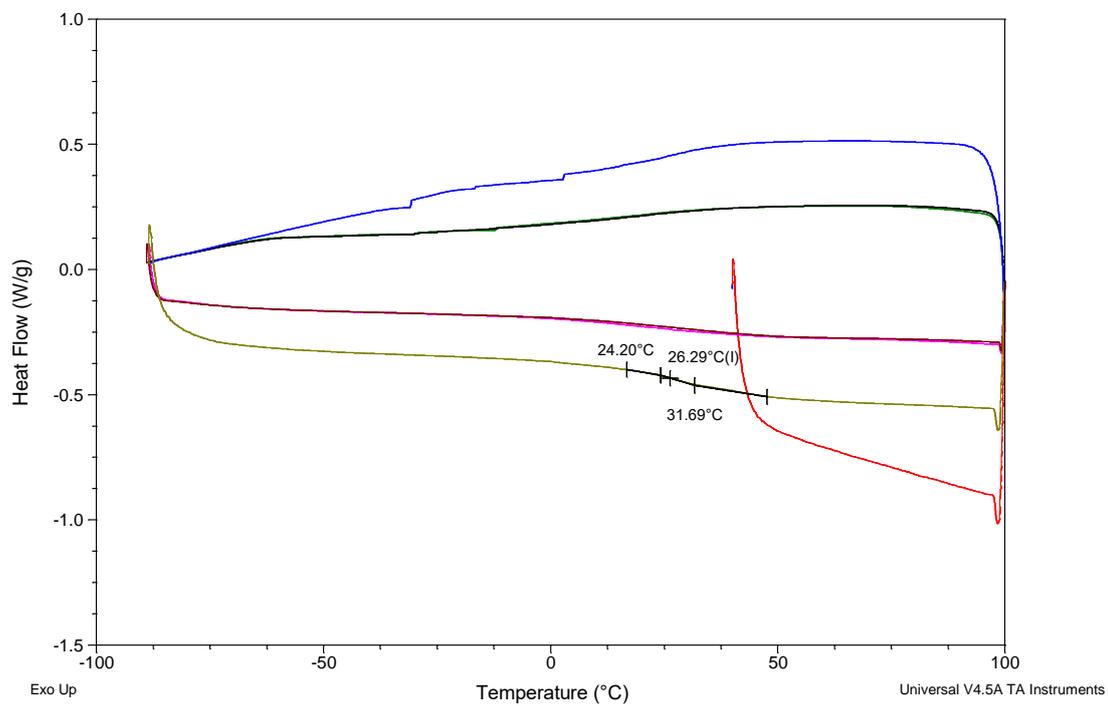


Figure S41. DSC thermogram of [HCQH₂][*p*-TolSO₃]₂.

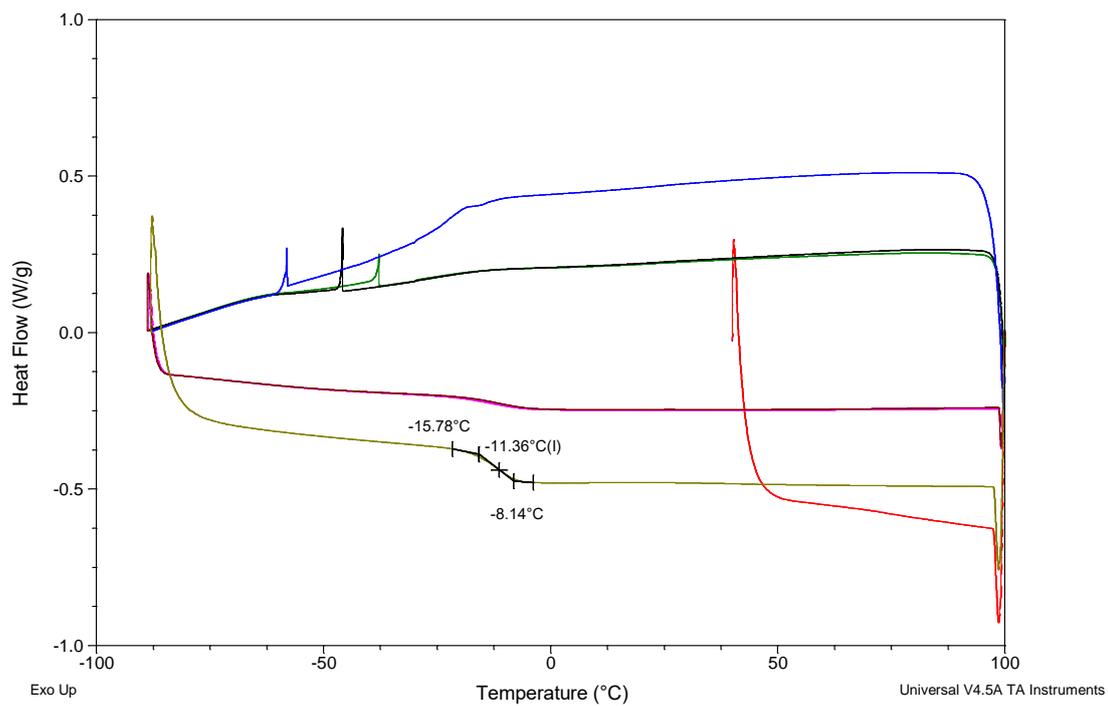


Figure S42. DSC thermogram of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$.

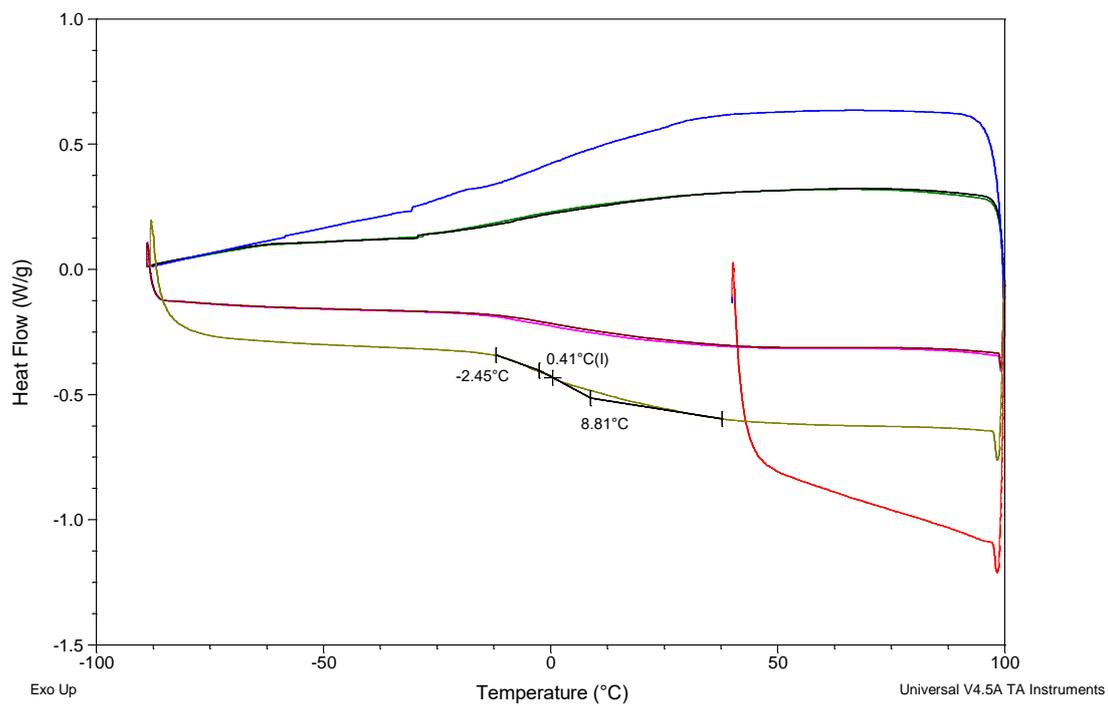


Figure S43. DSC thermogram of $[\text{HCQH}_2][\text{GlcCOO}]_2$.

Critical micelle concentrations

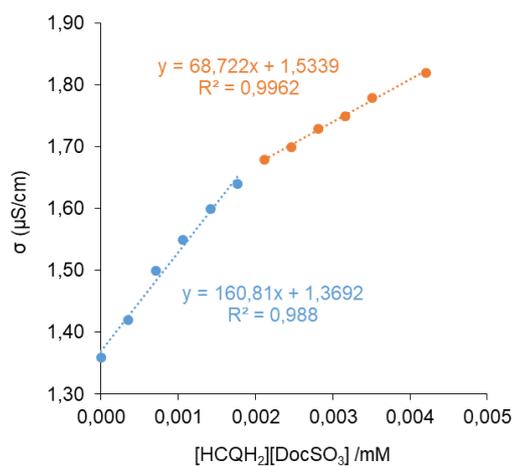


Figure S44. Plot of conductivity *vs* concentration of $[\text{HCQH}_2][\text{DocSO}_3]_2$ (5).

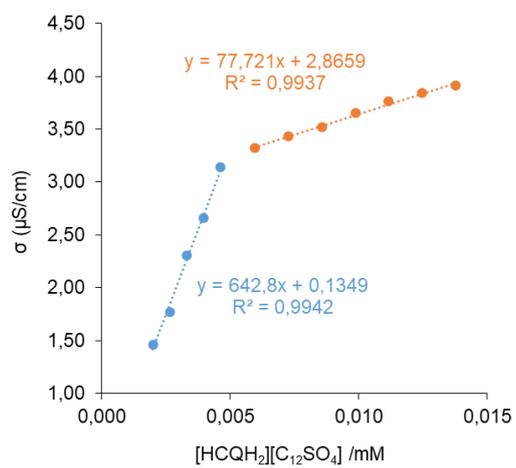


Figure S45. Plot of conductivity *vs* concentration of $[\text{HCQH}_2][\text{C}_{12}\text{SO}_4]_2$ (8).