Supplementary information

Lithium-Selective Supramolecular Assembly and Capture by Tripeptide Gelators

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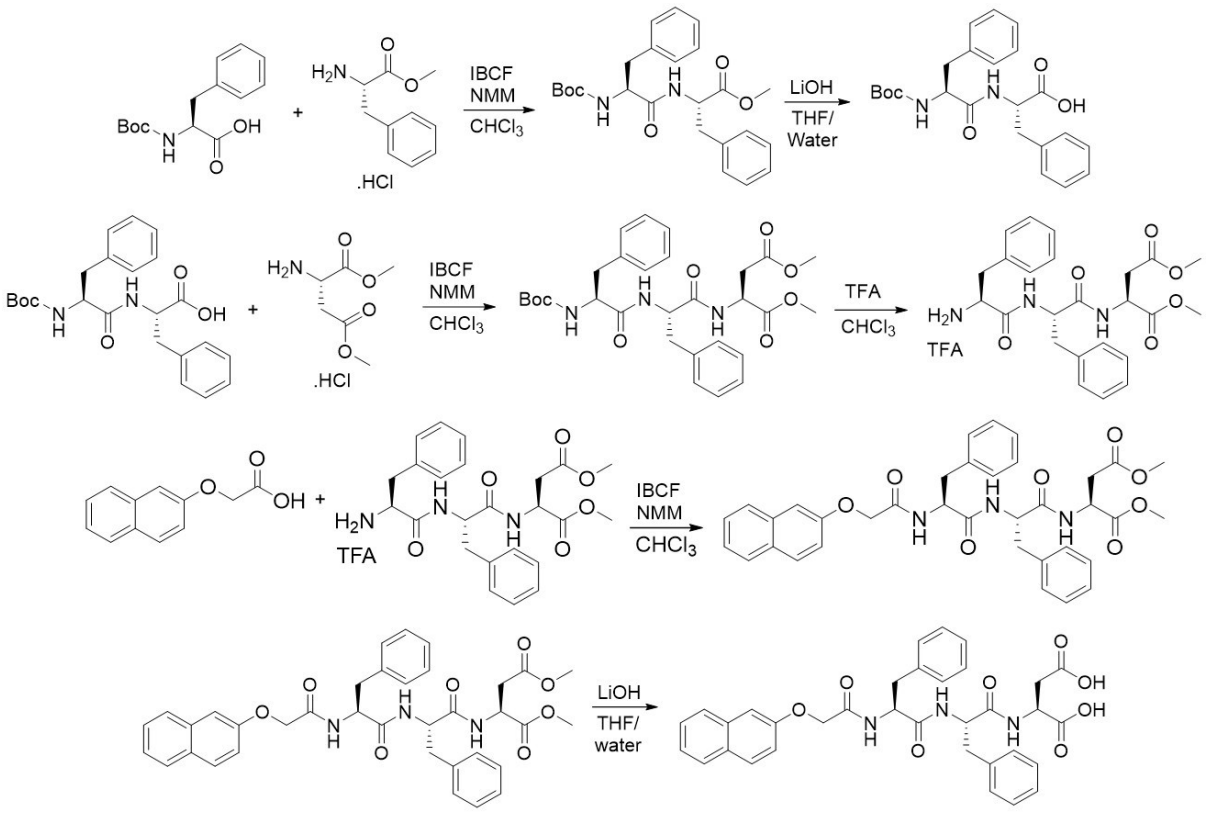
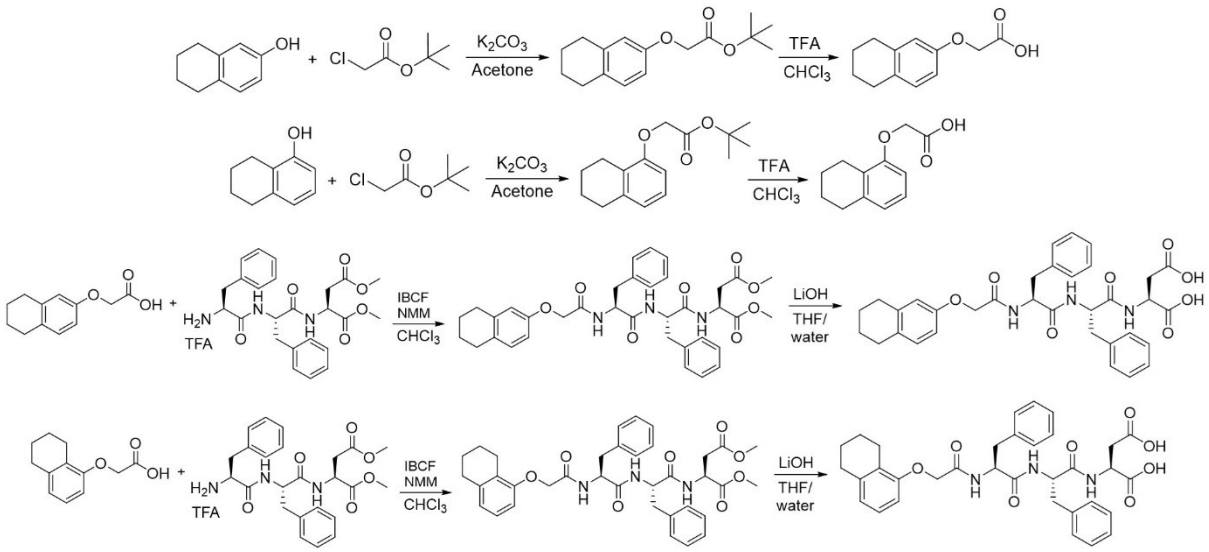


Scheme S1: Full synthetic route of the tripeptide gelator 2NapFFD.



Scheme S2: Full synthetic route of the tripeptide gelators 2ThNapFFD and 1ThNapFFD.

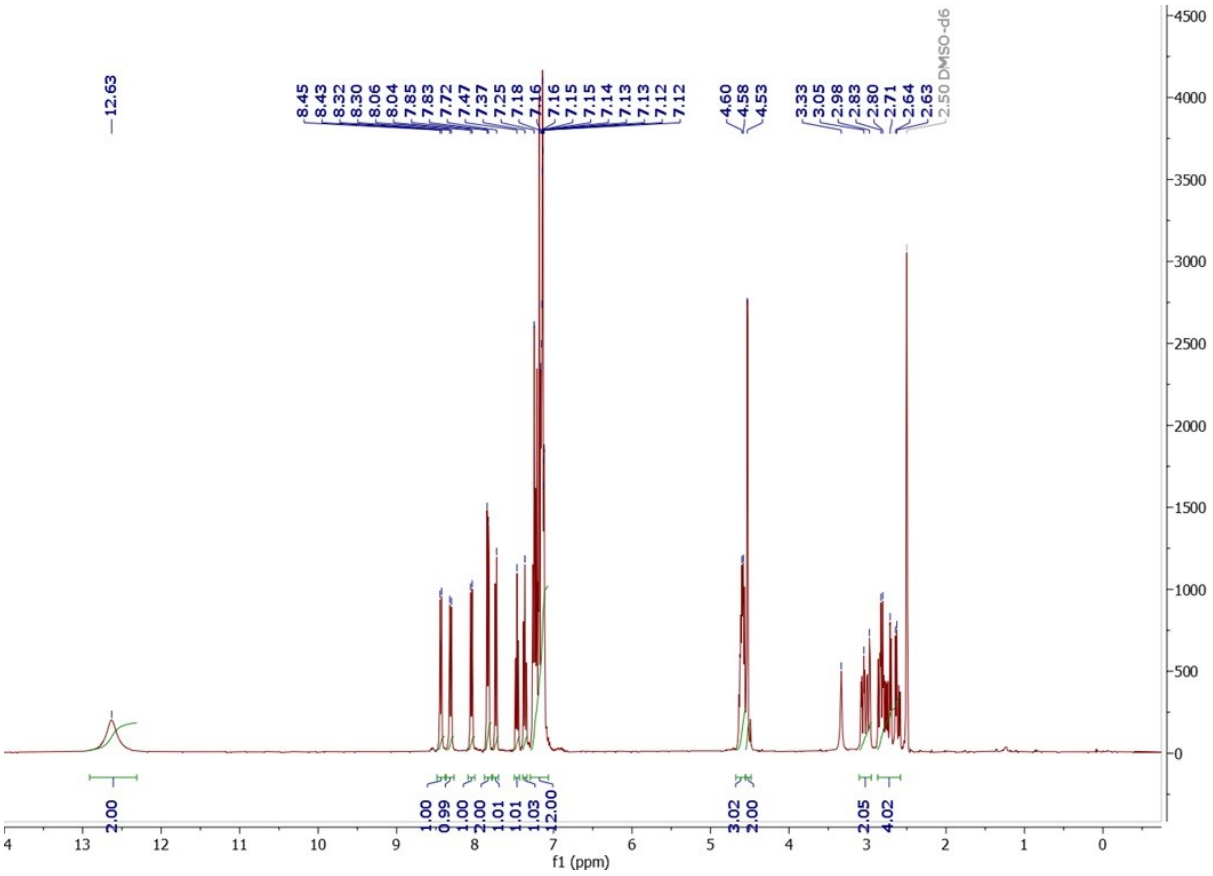


Figure S1: ^{1}H-NMR of *2NapFFD.*

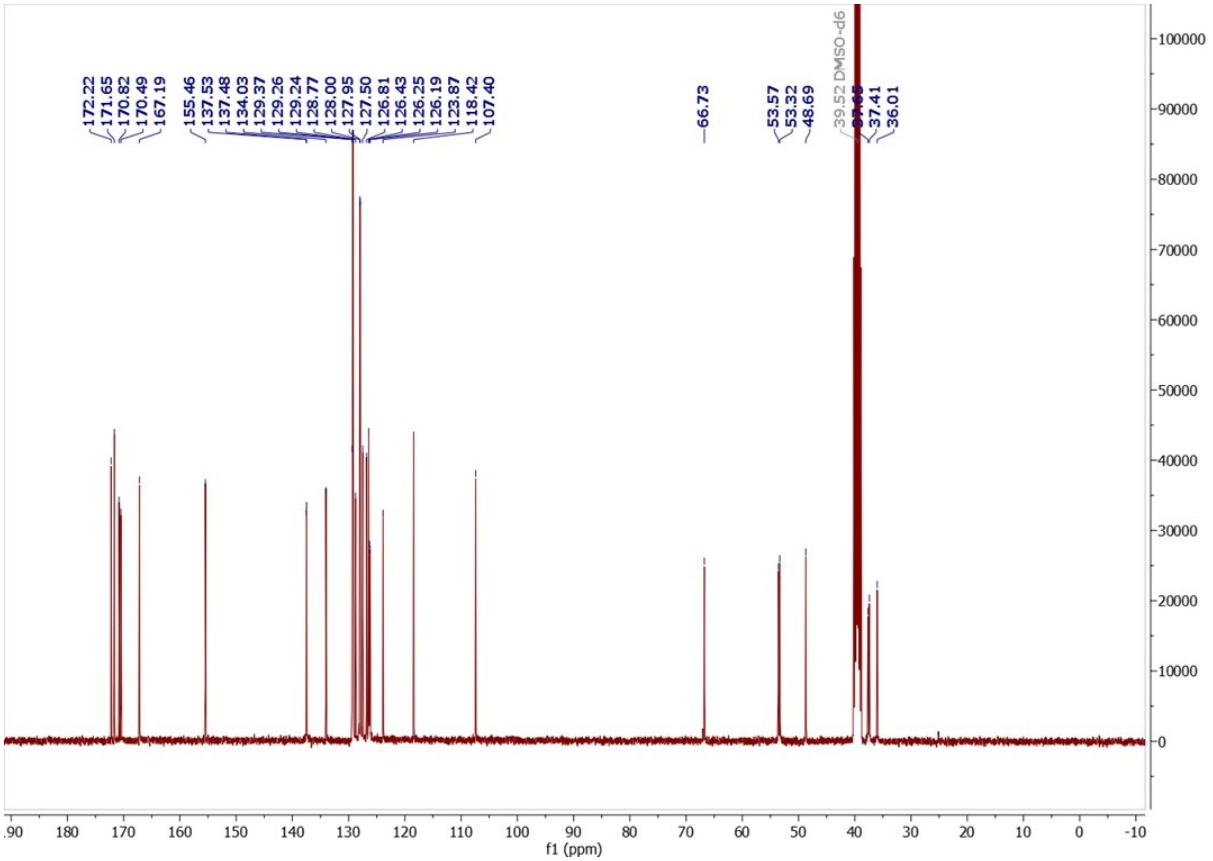


Figure S2: ^{13}C-NMR of *2NapFFD*.

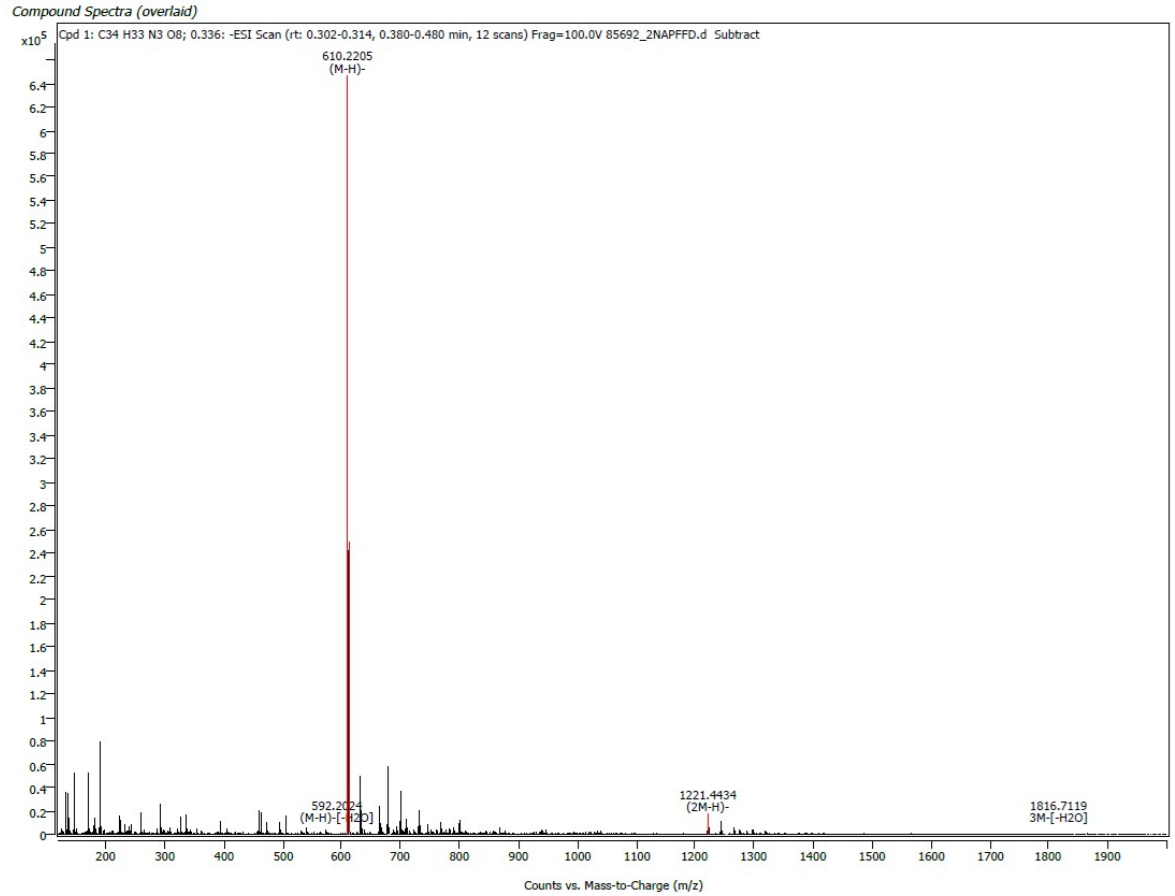


Figure S3: HRMS of *2NapFFD*.

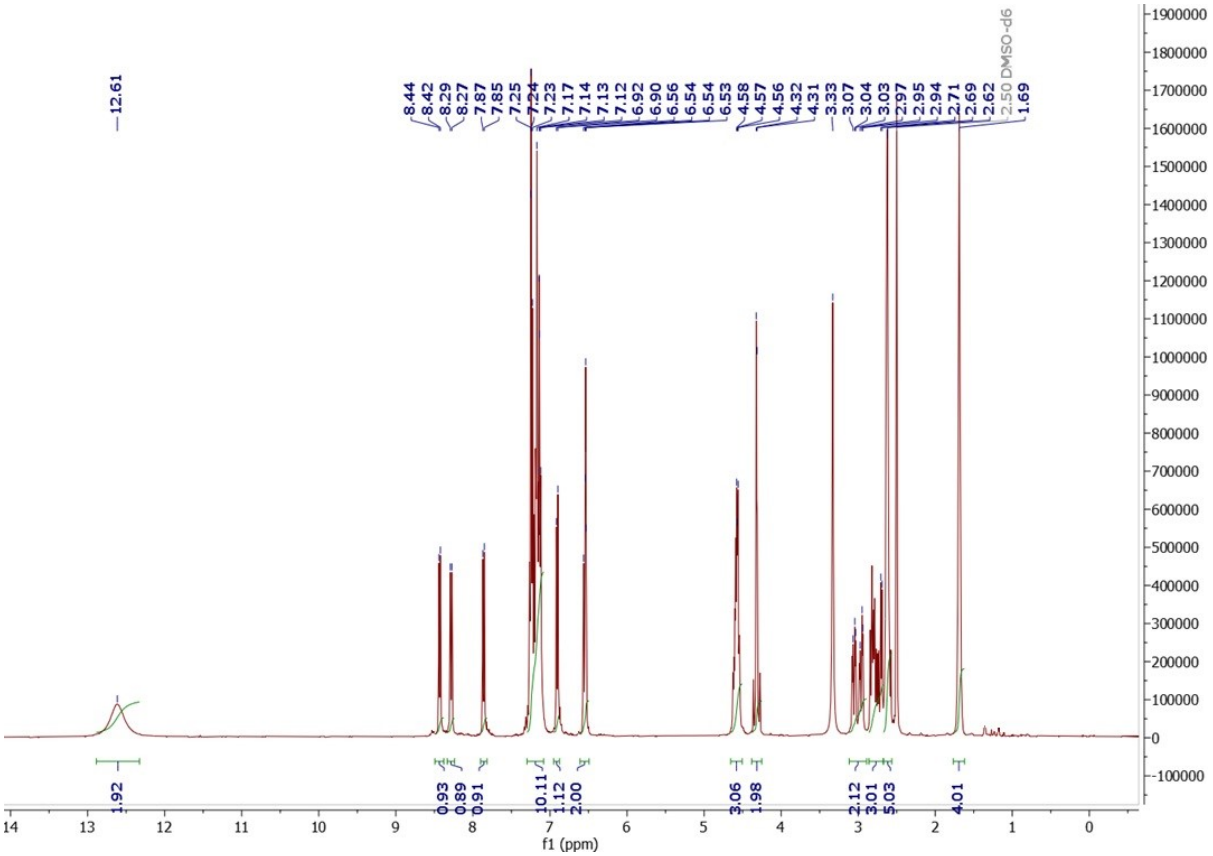


Figure S4: [1]H-NMR of *2ThNapFFD*.

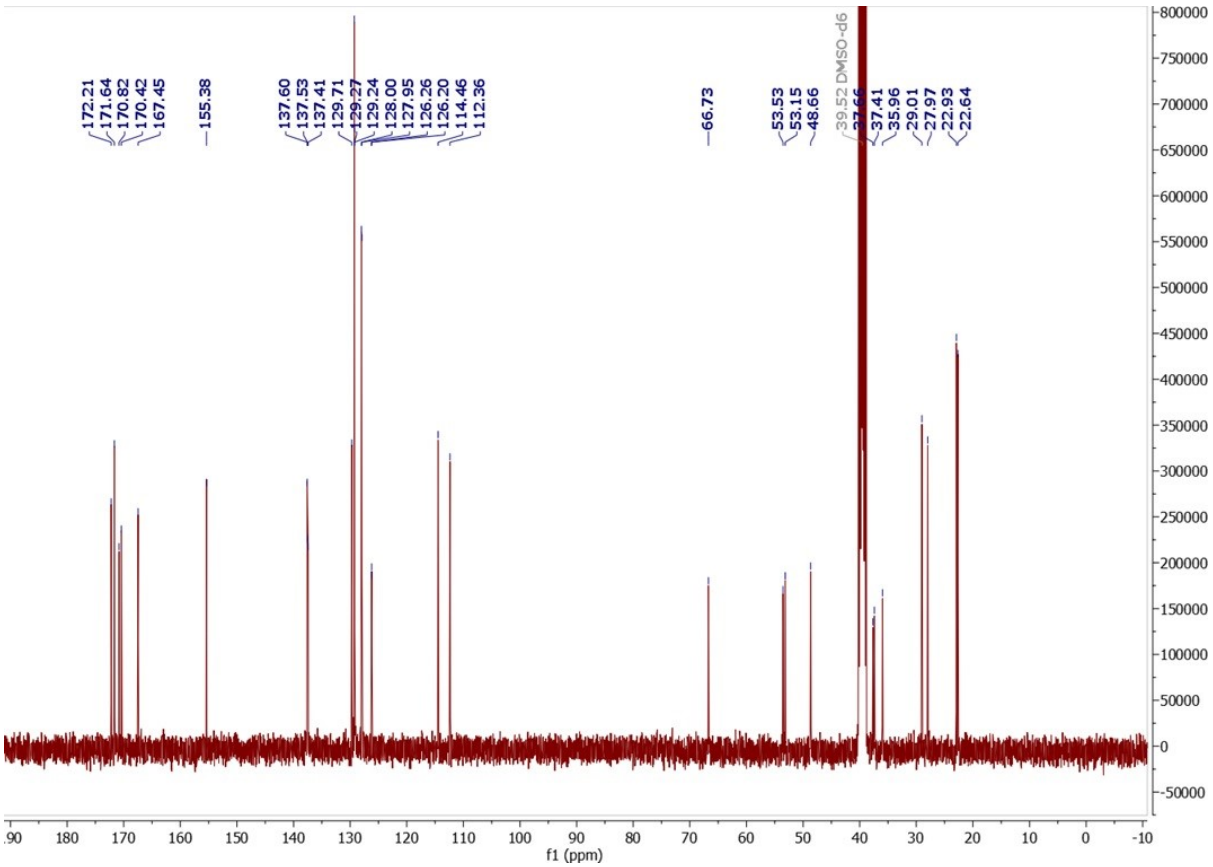


Figure S5: [13]C-NMR of *2ThNapFFD*.

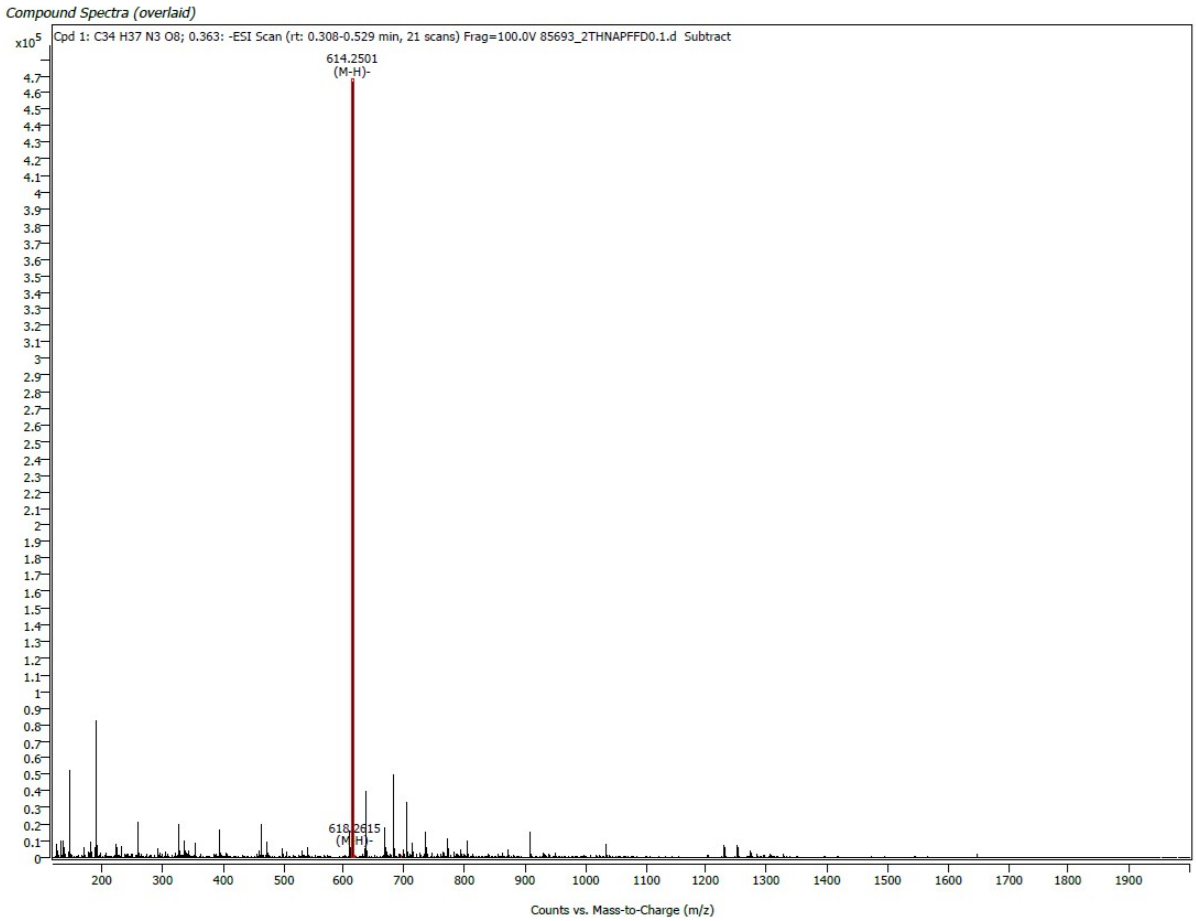


Figure S6: HRMS of *2ThNapFFD.*

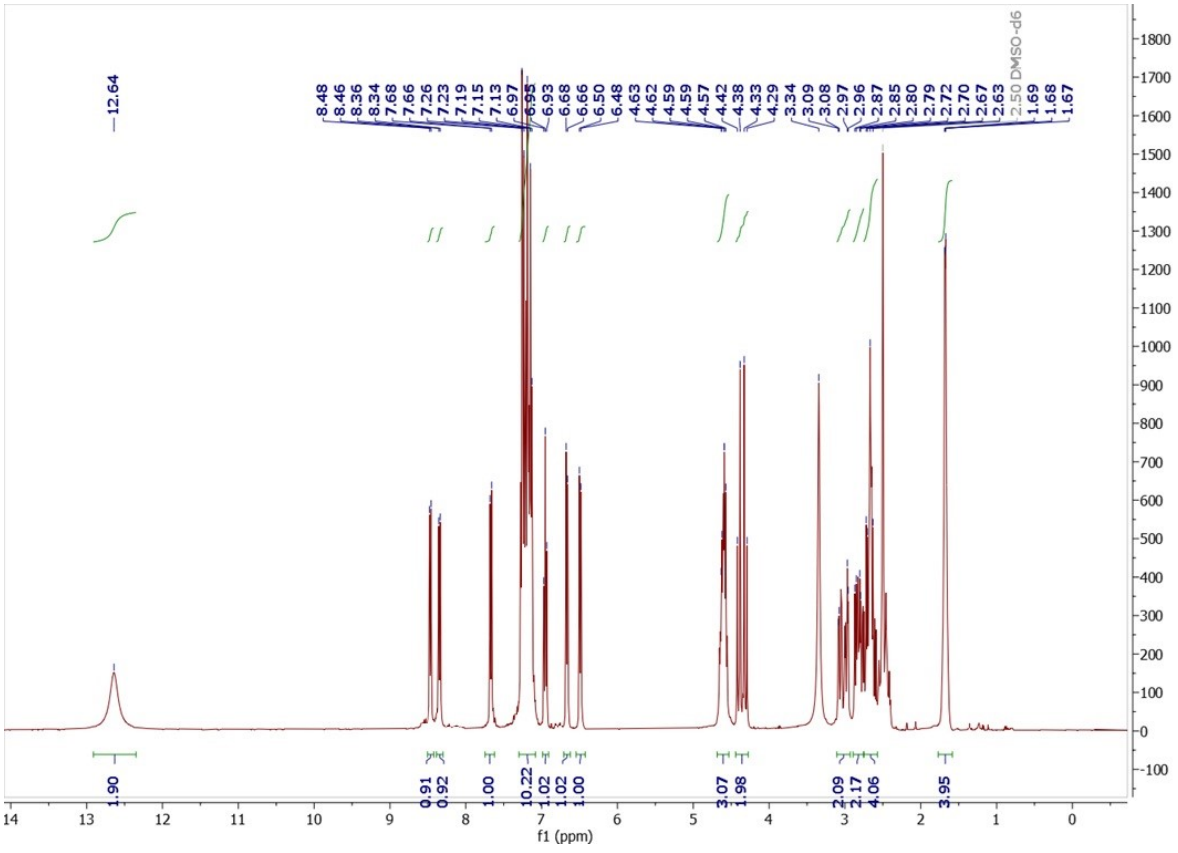


Figure S7: [1]H-NMR of *1ThNapFFD.*

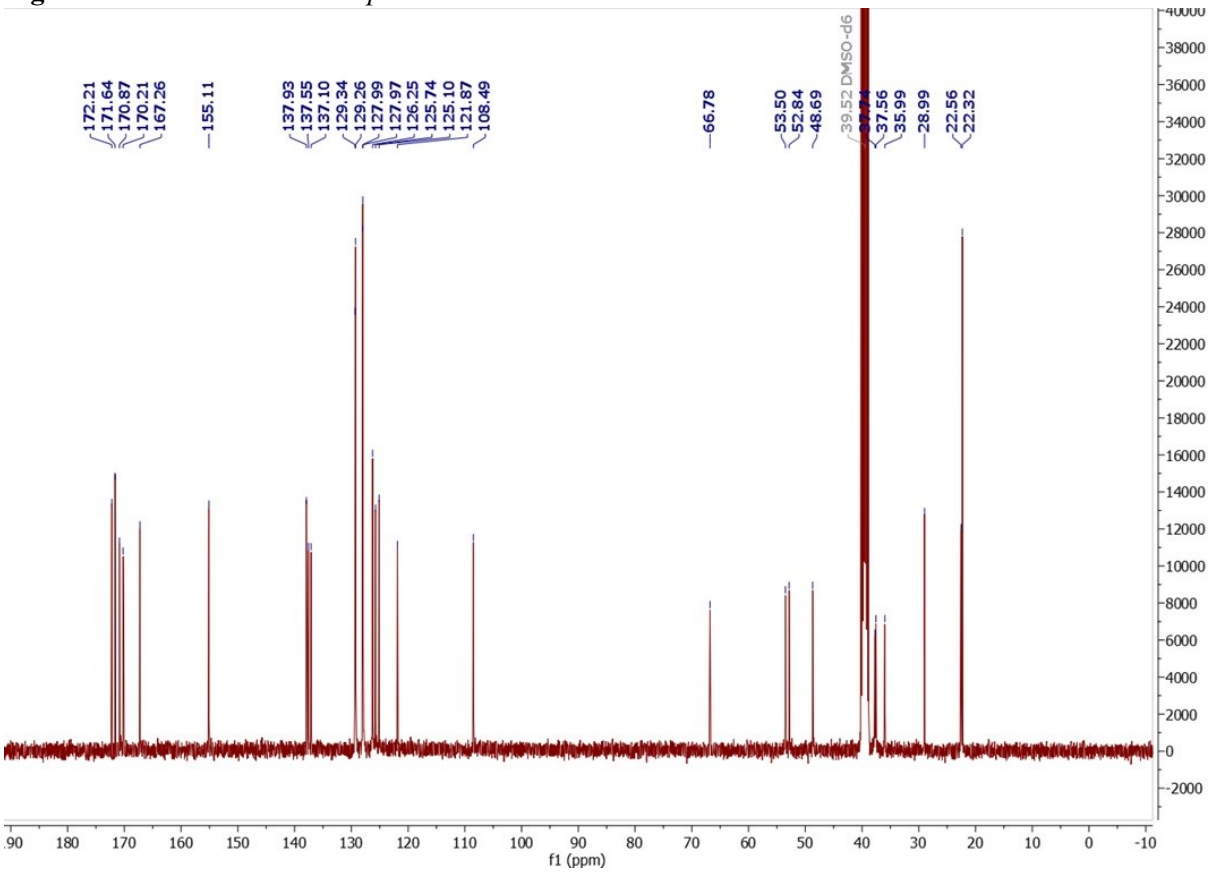


Figure S8: [13]C-NMR of *1ThNapFFD.*

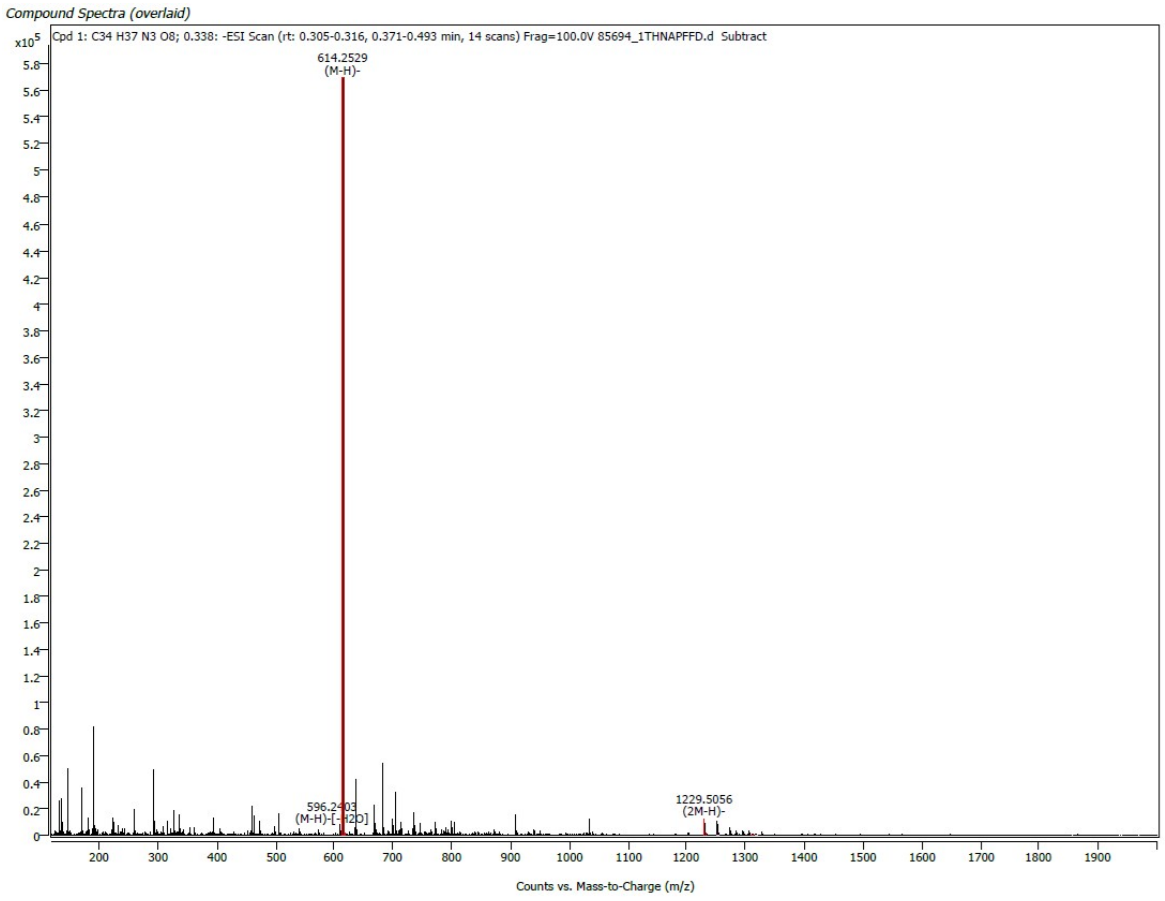


Figure S9: HRMS of *1ThNapFFD.*

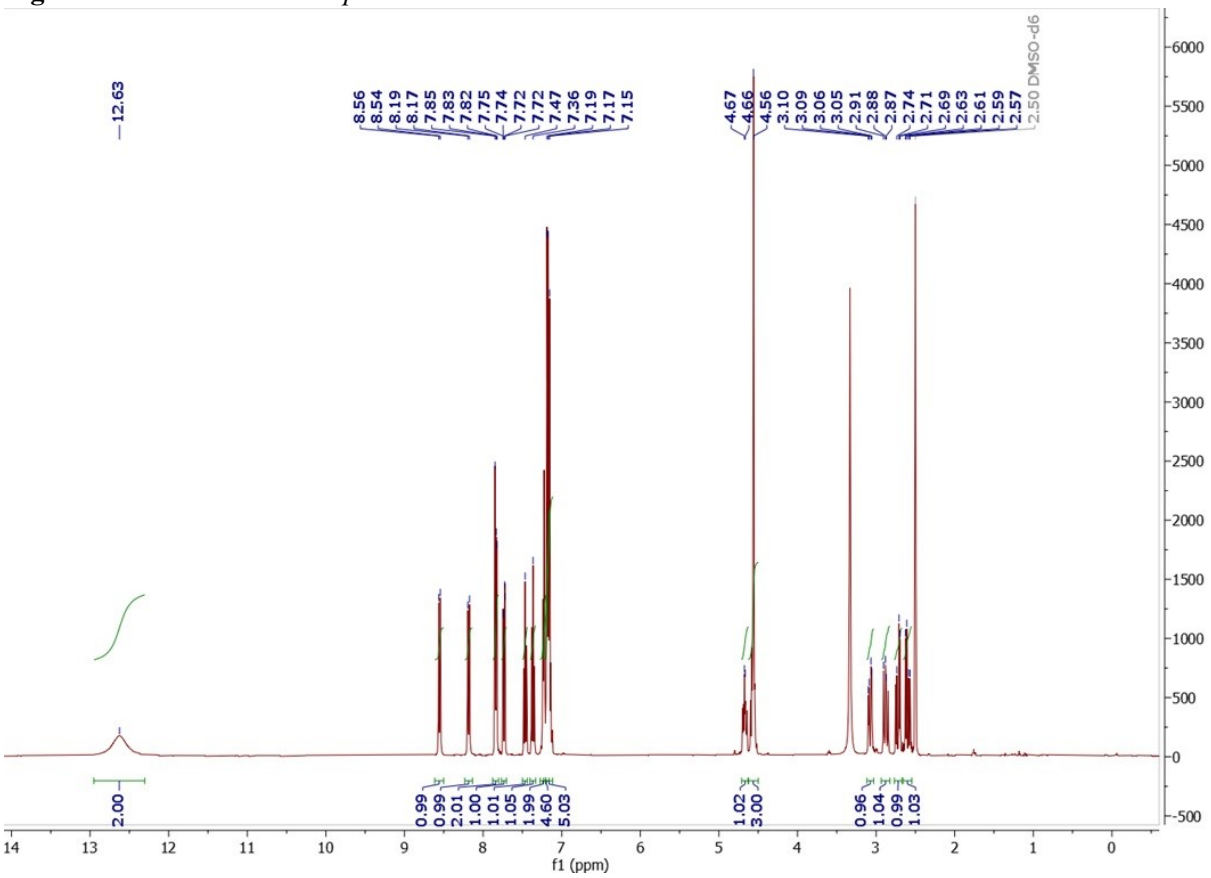


Figure S10: [1]H-NMR of *2NapFD.*

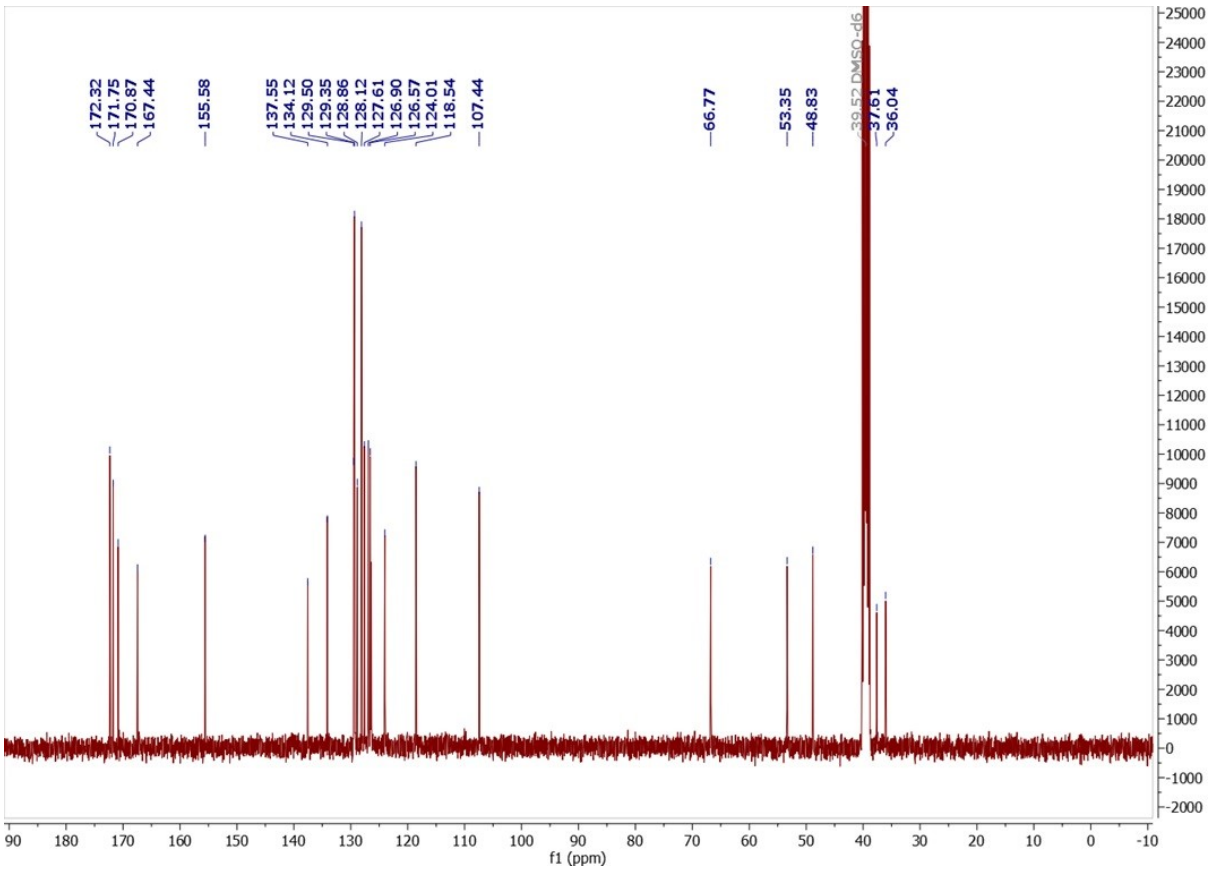


Figure S11: ^{13}C-NMR of *2NapFD.*

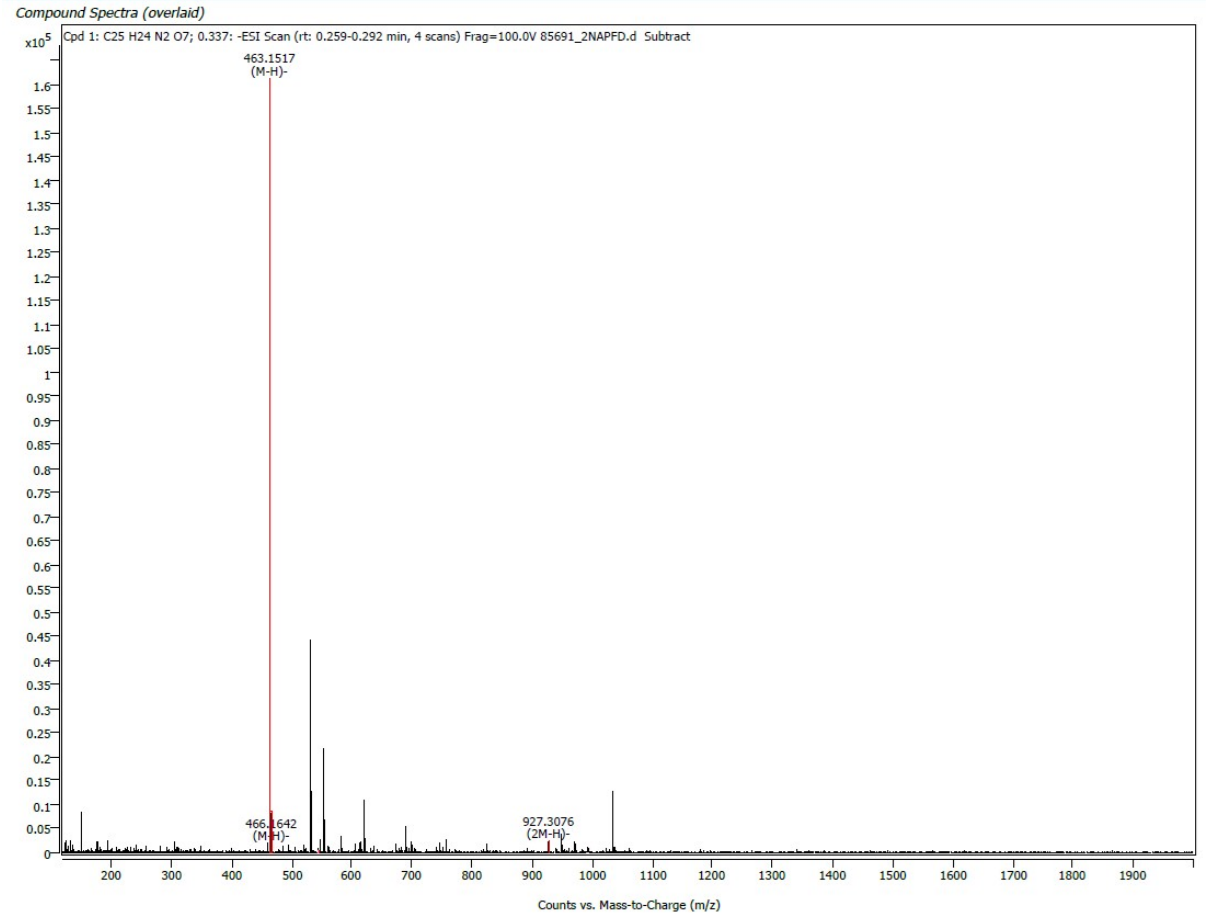


Figure S12: HRMS of *2NapFD.*

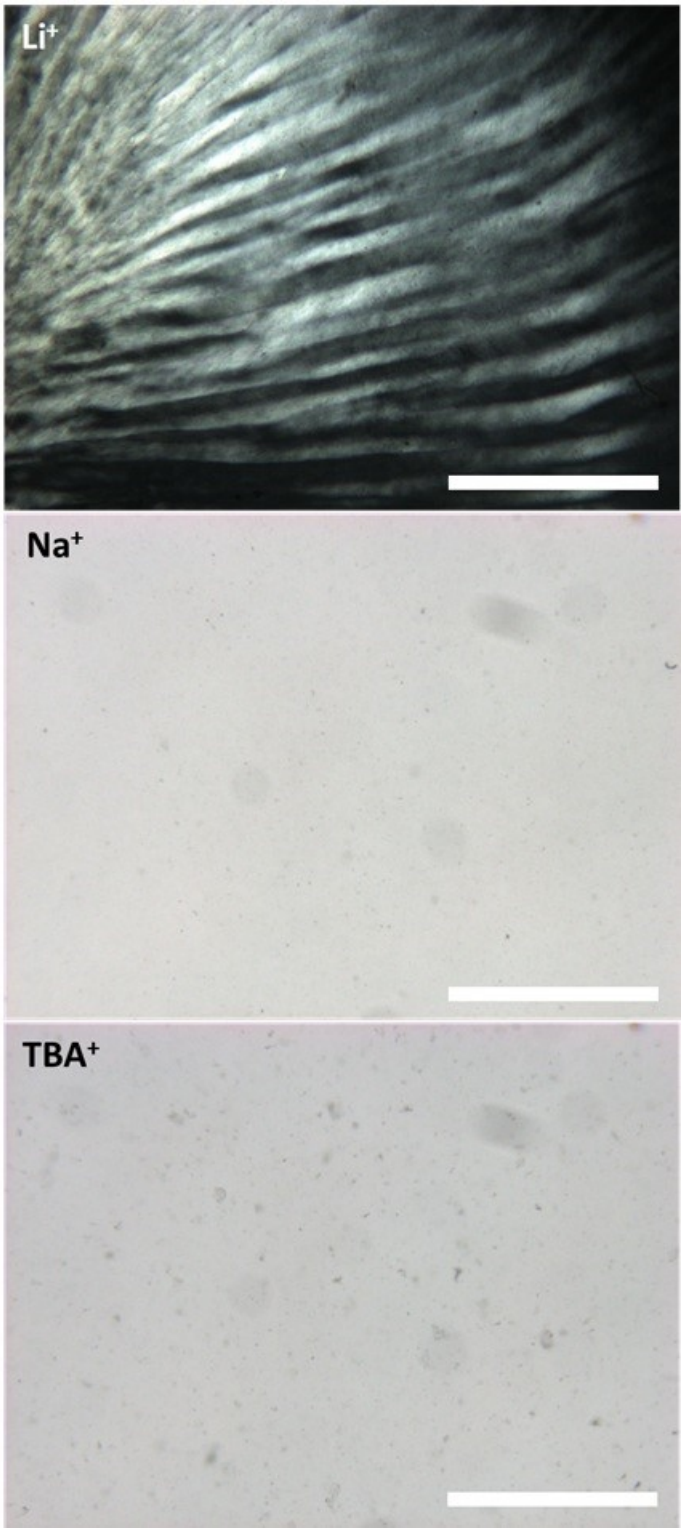


Figure S13: Microscopic images of 2NapFFD solutions prepared with Li^+, Na^+, and TBA^+ counterions (20 mg/mL, pH 10.5). The Li^+ sample is shown under polarised light (top), while the Na^+ and TBA^+ samples are brightfield images (middle and bottom). The polarised images of 2NapFFD·Na and 2NapFFD·TBA appeared completely black. Scale bars: 500 μm.

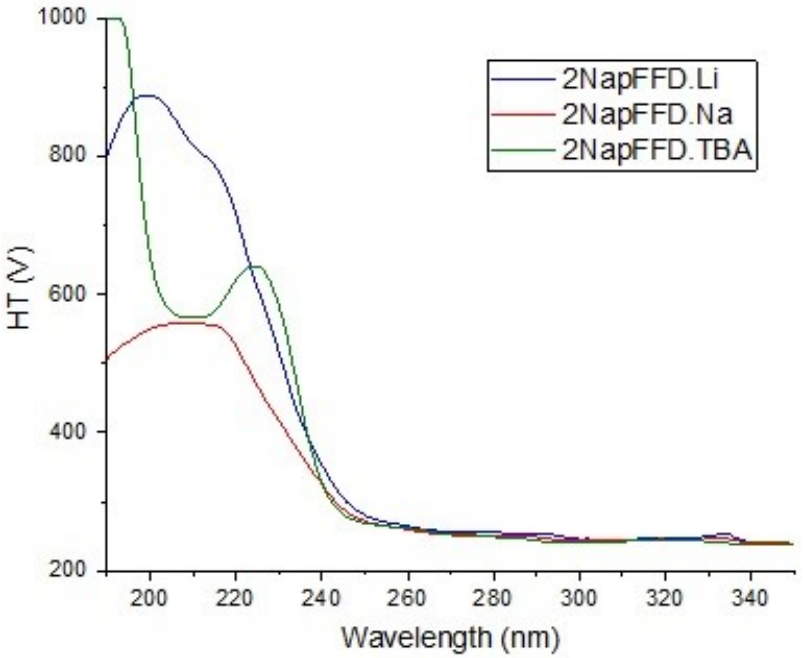


Figure S14: HT trace recorded during CD measurements of 2NapFFD solutions prepared with Li^+, Na^+, and TBA^+ counterions (20 mg/mL, pH 10.5).

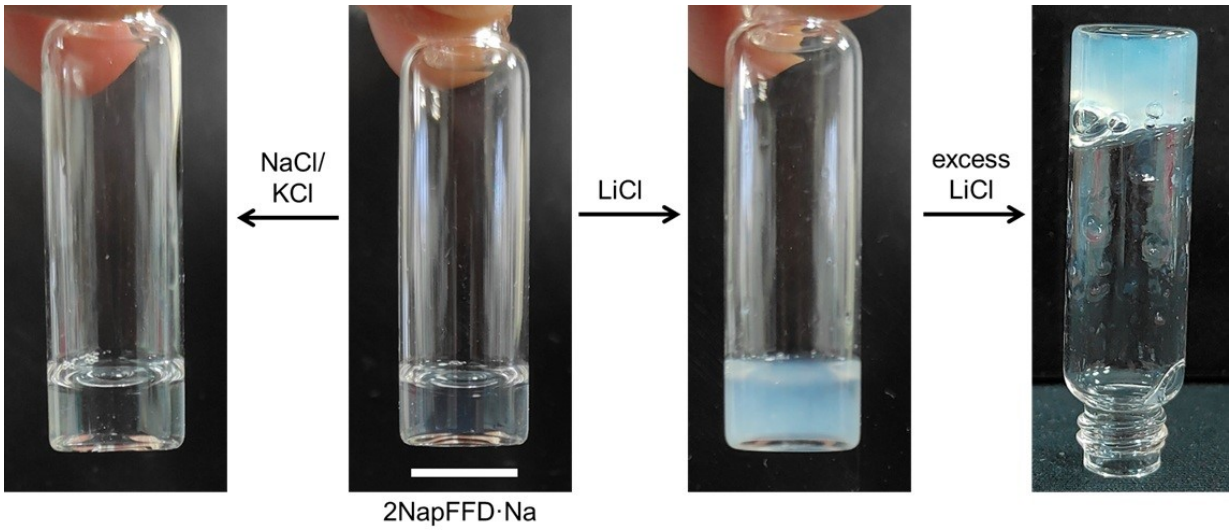


Figure S15: Photographs showing ion-selective response of 2NapFFD. Adding NaCl or KCl to 2NapFFD·Na solution (20 mg/mL, pH 10.5) produces no visible change, whereas adding LiCl induces significant thickening and further excess LiCl yields a self-supporting gel (tested by vial inversion). Scale bar: 1 cm.

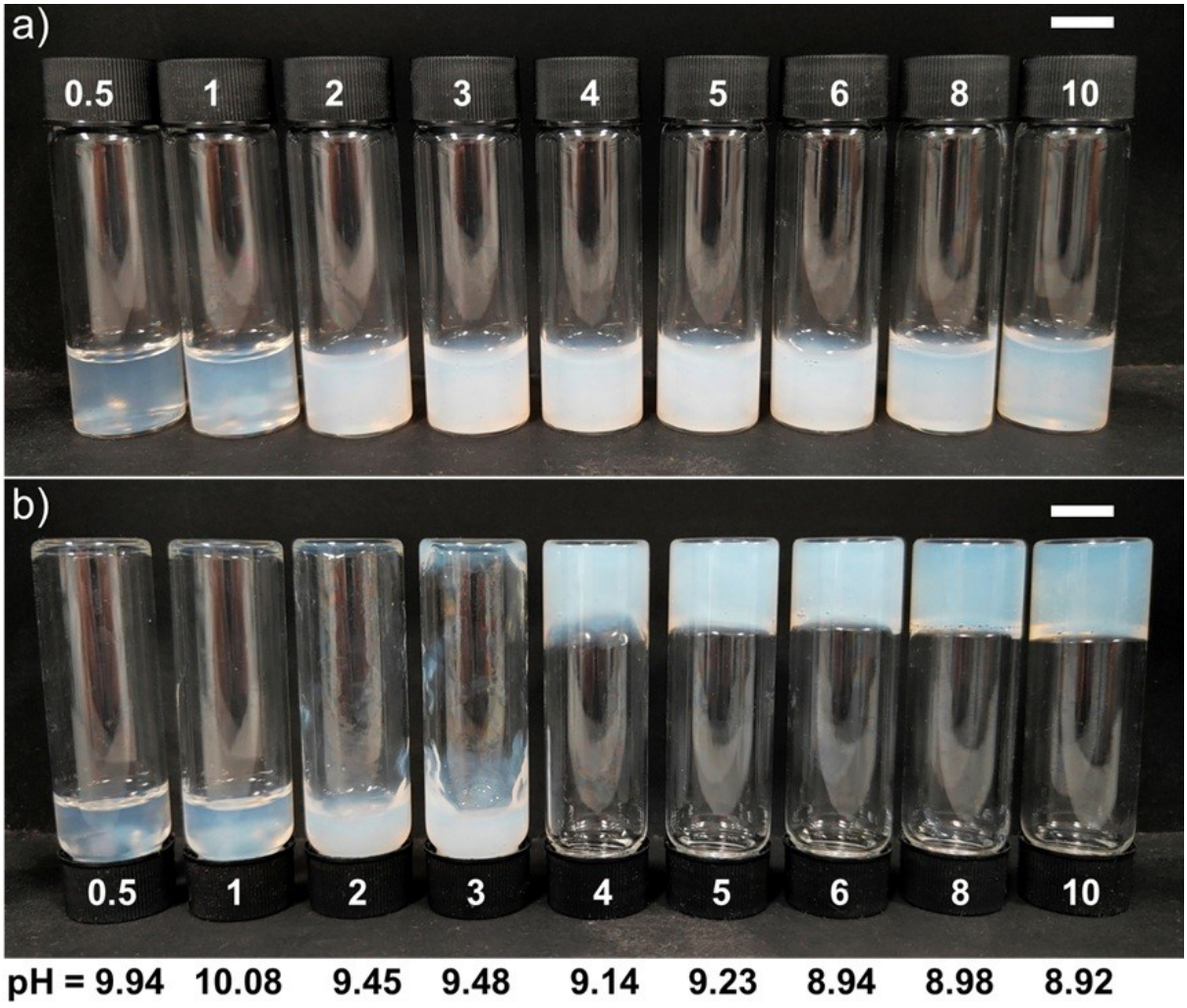


Figure S16: Photographs of 2NapFFD·Na solutions (20 mg/mL, pH 10.5) after addition of increasing equivalents of solid LiCl. The number of equivalents is shown on the vials. (a) Vials upright. (b) Vials after inversion, showing gel formation at higher LiCl equivalents. The final pH (after 24 h of mixing the LiCl) of the solutions are given below, showing basic pH for all the solutions. In the same time interval, the pH of the pure 2NapFFD·Na solution (without any added LiCl) drops to 10.28. Scale bars: 1 cm.

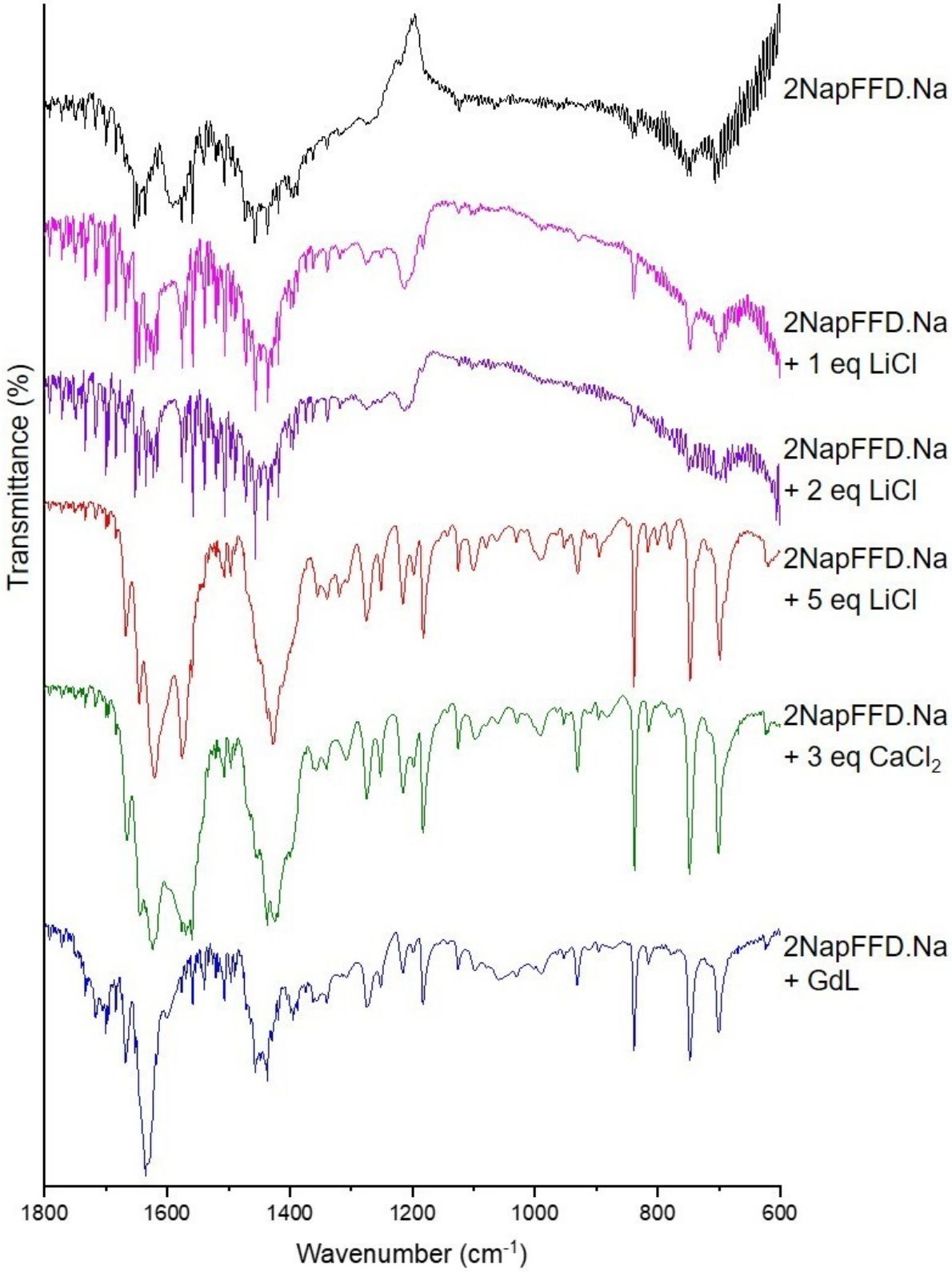


Figure S17: ATR-FTIR spectra recorded in D_2O for 2NapFFD.Na salt solution, 2NapFFD.Na + LiCl (1 and 2 eq) solutions, and gels formed from 2NapFFD.Na by addition of 5 eq LiCl, 3 eq $CaCl_2$, or GdL. The LiCl- and $CaCl_2$-triggered gels show broadly similar spectral profiles, whereas the GdL-triggered gel shows a distinct profile, consistent with differences in protonation state and local hydrogen-bonding environment. The corresponding solution spectra were noisy, likely because liquid

samples in D_2O give weaker ATR signals and less reproducible contact with the ATR crystal compared to the gel samples.

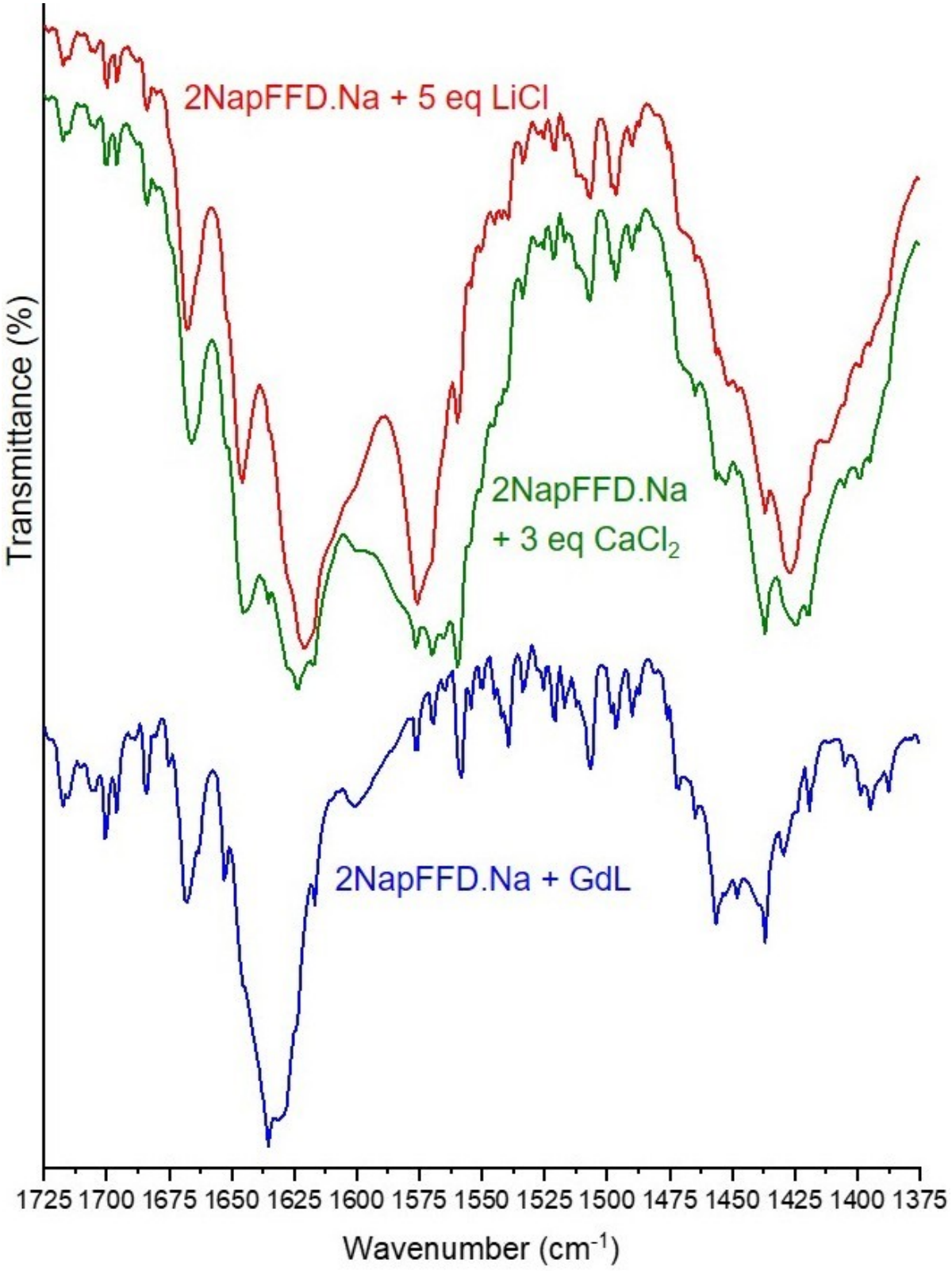


Figure S18: Expanded ATR-FTIR spectra of the amide/carboxylate region for gels formed from 2NapFFD.Na by addition of 5 eq LiCl, 3 eq $CaCl_2$, or GdL in D_2O.

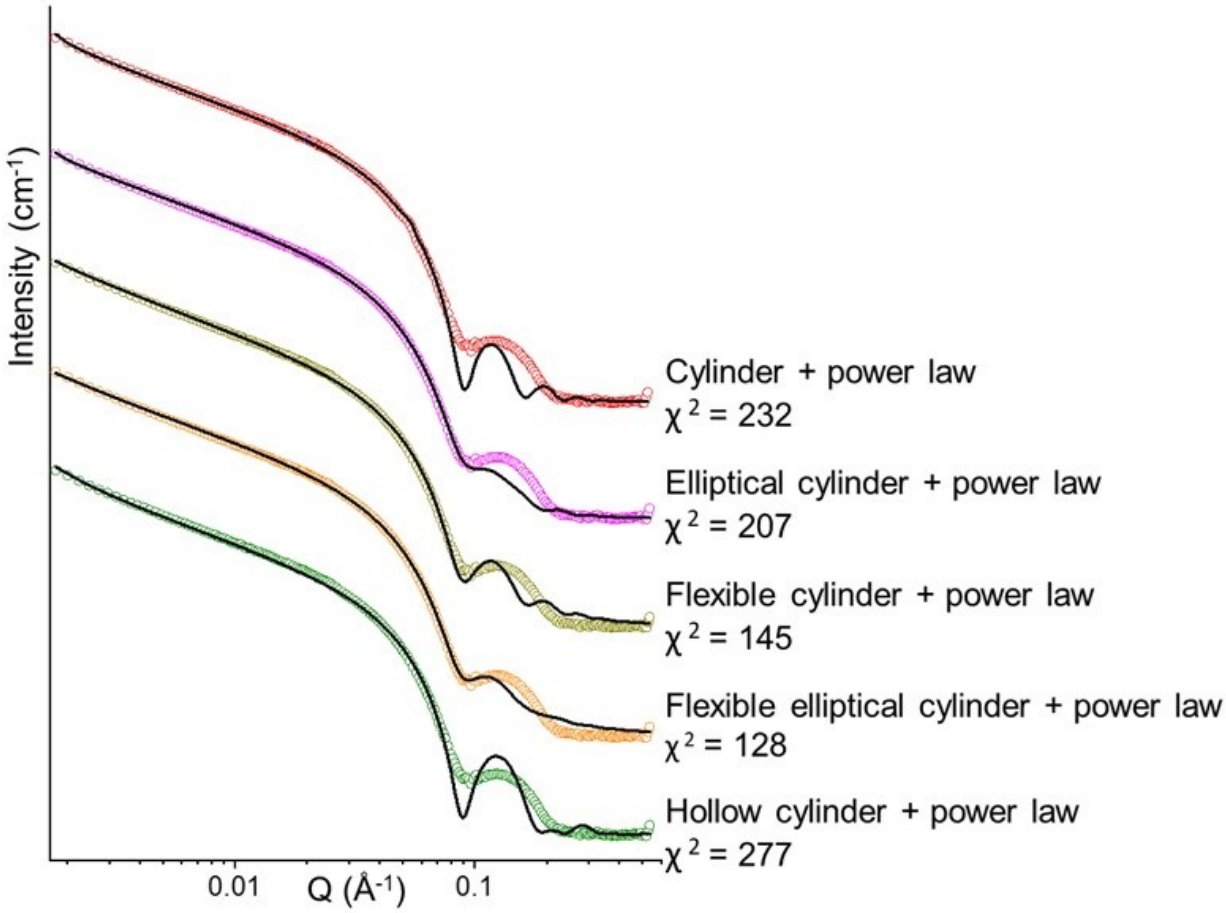


Figure S19: Fits obtained for 2NapFFD.Na (20 mg/mL, pD 10.9) + 2 eq LiCl with single cylindrical models and power law, corresponding χ^2 values are provided adjacent to the fit. Similar fittings were obtained in all 2NapFFD/2ThNapFFD.Li samples.

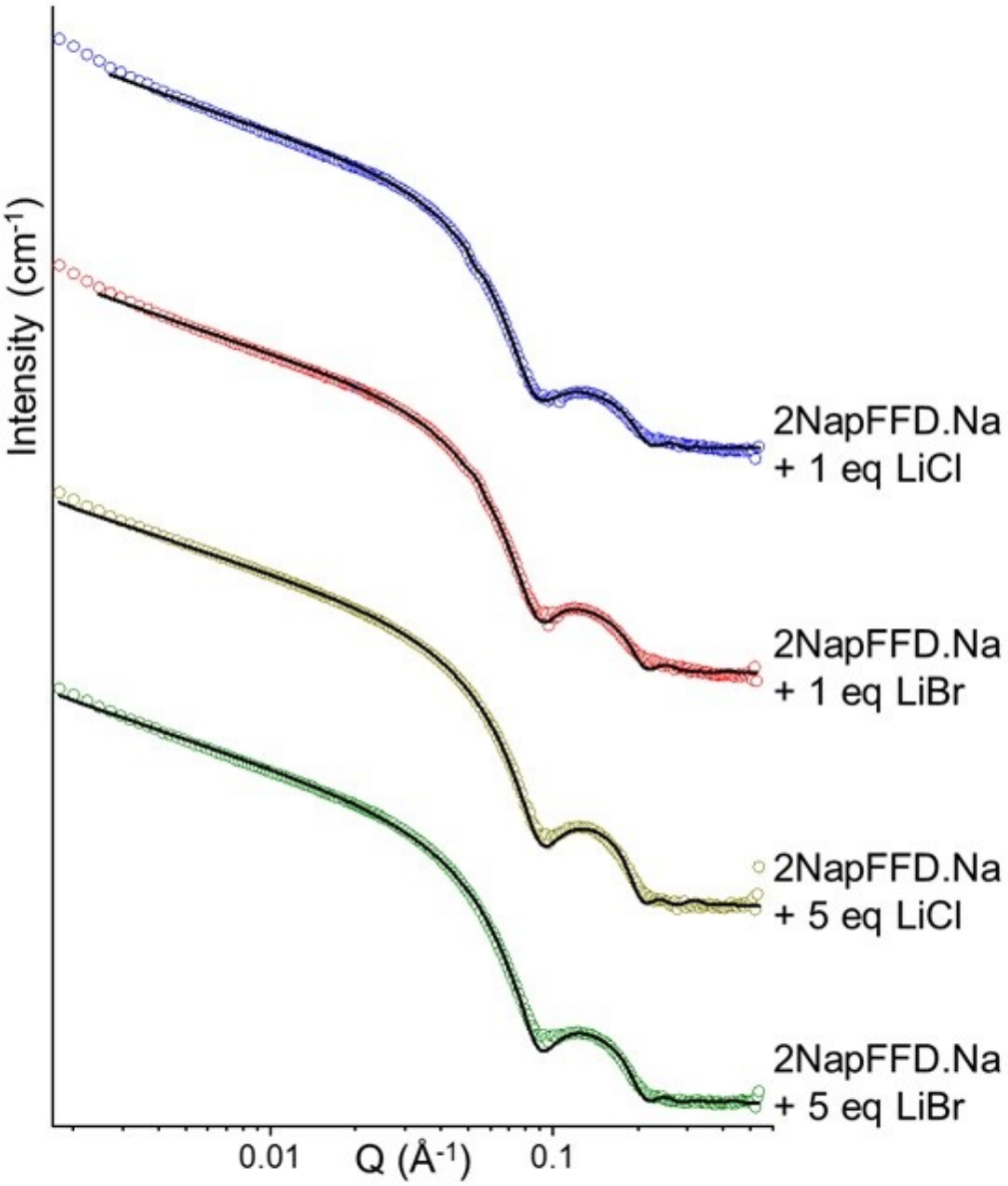


Figure S20: SANS profiles of 2NapFFD·Na (20 mg/mL, pD 10.9, D_2O) after adding 1 and 5 equivalents of LiCl and LiBr, showing similar scattering patterns.

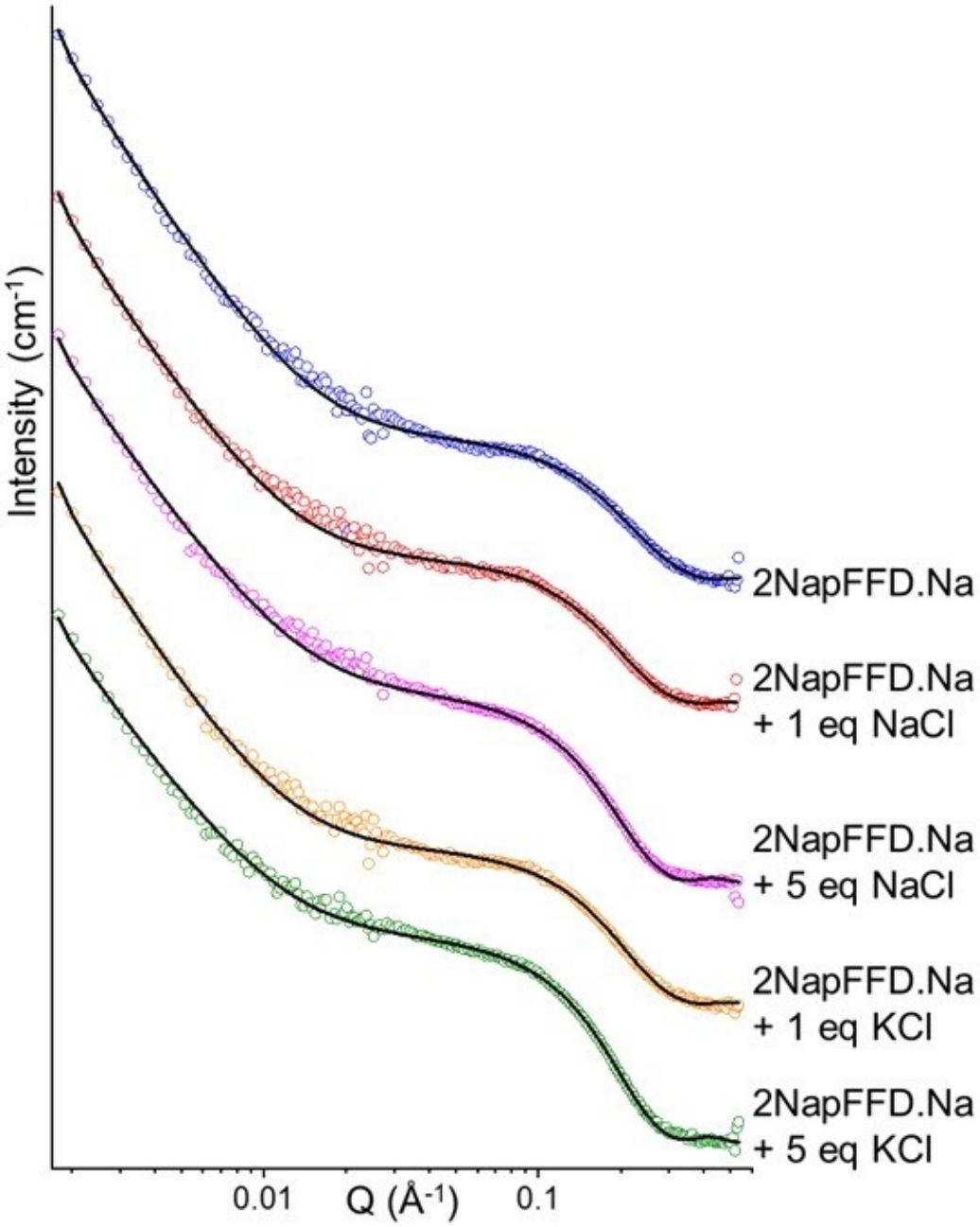


Figure S21: SANS profiles of 2NapFFD·Na (20 mg/mL, pD 10.9, D_2O) after adding 1 and 5 equivalents of NaCl and KCl, showing no change in scattering patterns.

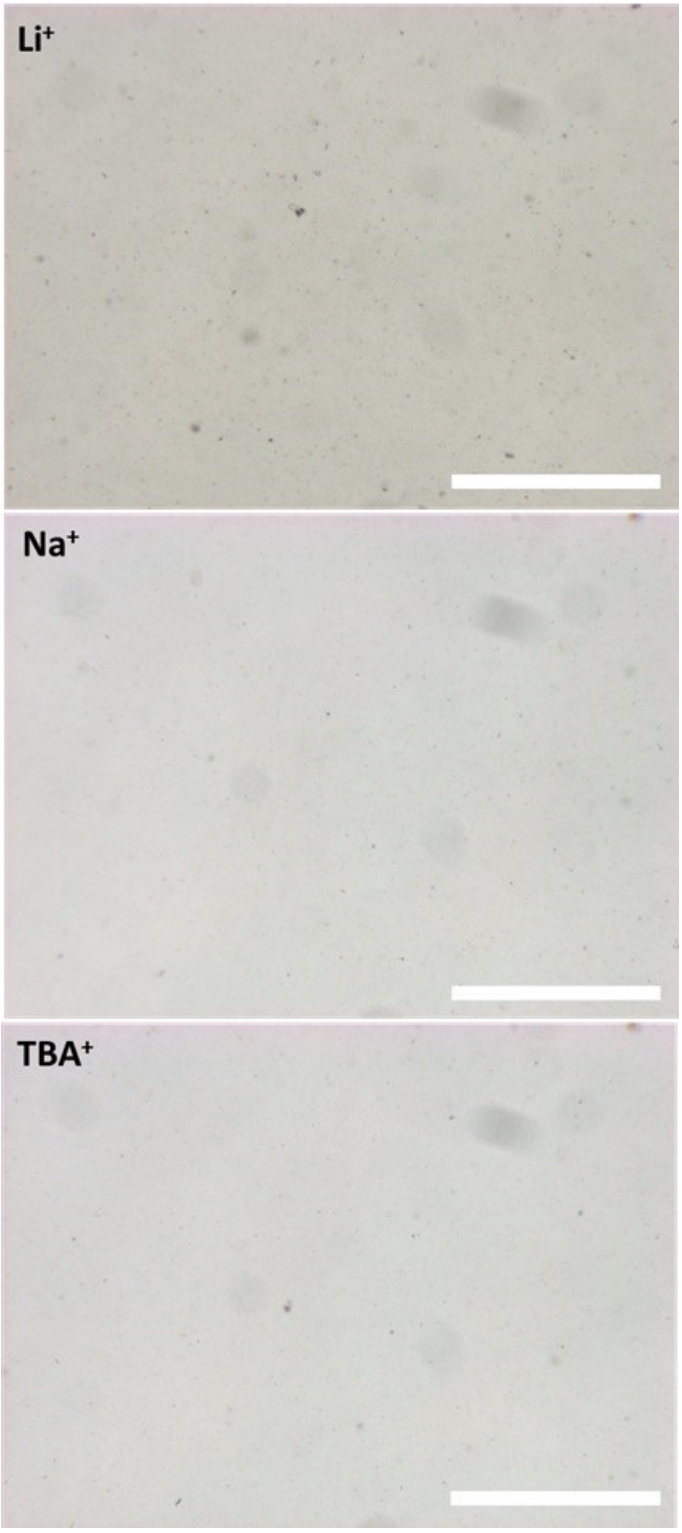


Figure S22: Brightfield optical micrographs of 2ThNapFFD solutions prepared with Li^+, Na^+, and TBA^+ counterions (20 mg/mL, pH 10.5). The polarised images of all the solutions appeared completely black. Scale bars: 500 μm.

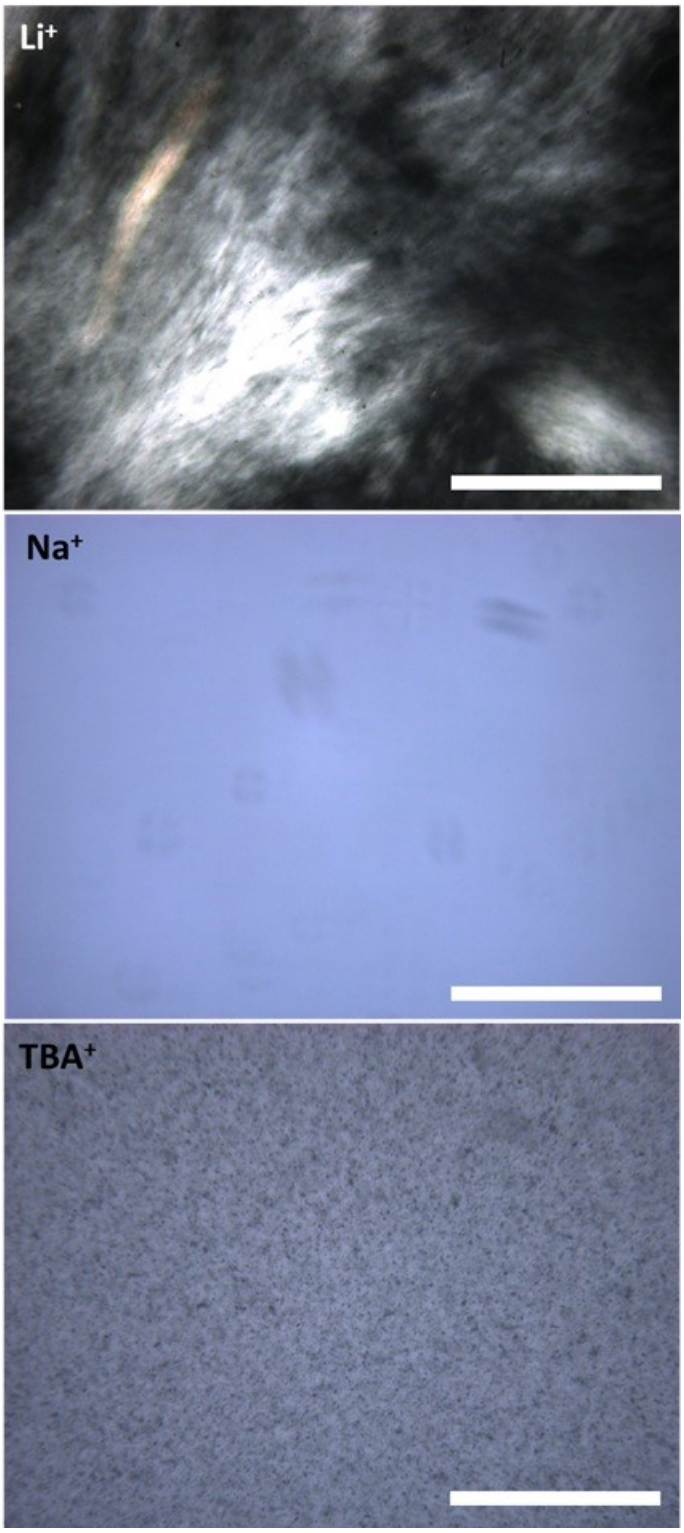


Figure S23: Microscopic images of 1ThNapFFD solutions prepared with Li^+, Na^+, and TBA^+ counterions (20 mg/mL, pH 10.5). The Li^+ sample is shown under polarised light (top), while the Na^+ and TBA^+ samples are brightfield images (middle and bottom). The polarised images of 1ThNapFFD·Na and 1ThNapFFD·TBA appeared completely black. Scale bars: 500 µm.

Table S1. Fitting parameters for SAXS data of 2NapFFD salts with counterions other than Li

Counterions	Na	K	Rb	Cs	TBA	BTMA
Model	Cylinder + Power law					
Background (cm^{-1})	0.00043 ± 0.00021	0.0029 ± 0.0022	0.00625 ± 0.00086	0.01217 ± 0.00062	0.003	0.002
A Scale	0.00183 ± 0.00073	$1.41 \times 10^{-6} \pm 4.07 \times 10^{-7}$	0.00181 ± 0.00016	$0.00226 \pm 8.95 \times 10^{-5}$	0.00127 ± 0.00010	$0.00203 \pm 9.12 \times 10^{-5}$
A Length (Å)	46.4 ± 3.4	203 ± 22	50.9 ± 2.0	56.8 ± 1.3	26.1 ± 2.8	26.9 ± 1.8
A Radius (Å)	9.0 ± 1.7	7.2 ± 2.5	11.8 ± 0.6	13.3 ± 0.3	15.1 ± 3.3	15.6 ± 2.3
B Scale	$2.82 \times 10^{-6} \pm 5.19 \times 10^{-7}$	$7.58 \times 10^{-7} \pm 3.44 \times 10^{-7}$	$4.89 \times 10^{-7} \pm 1.59 \times 10^{-8}$	$2.51 \times 10^{-7} \pm 2.36 \times 10^{-9}$	$2.82 \times 10^{-8} \pm 7.43 \times 10^{-10}$	$2.06 \times 10^{-7} \pm 2.30 \times 10^{-9}$
B Power	2.55 ± 0.03	2.78 ± 0.08	3.28 ± 0.01	3.69 ± 0.00	3.89 ± 0.00	3.66 ± 0.00
χ^2	0.49	0.41	0.55	2.96	0.86	5.92

Table S2. Fitting parameters for SAXS data of 2NapFFD.Li solution

	2NapFFD.Li
Model	Cylinder + Hollow cylinder
Background (cm^{-1})	0.0052 ± 0.0003
A Scale	$0.00242 \pm 1.09 \times 10^{-5}$
A Length (Å)	>1000
A Radius (Å)	55.3 ± 0.1
B Scale	$0.00183 \pm 5.26 \times 10^{-5}$
B Length (Å)	413 ± 9
B Radius (Å)	12.5 ± 0.0
B Thickness (Å)	20.2 ± 0.1
χ^2	4.34

Table S3. Fitting parameters for SAXS data of 2NapFFD solutions and GdL

Counterions	Li	Na	TBA
Model	Elliptical cylinder + Power law	Elliptical cylinder	Cylinder + Power law
Background (cm^{-1})	0.005	0.0020 ± 0.0003	0.00778 ± 0.00048
A Scale	0.0070 ± 3.17 $x10^{-6}$	0.007 ± 1.06 $x10^{-5}$	0.00484 ± 1.6 $x10^{-5}$
A Length (Å)	766 ± 3	>1000	144 ± 0.5
A Radius (Å)	45.1 ± 0.07	20.9 ± 0.03	32.0 ± 0.04
A Axis ratio	1.29 ± 0.004	5.52 ± 0.01	-
B Scale	2.48 $x10^{-11}$ ± 4.13 $x10^{-12}$	-	2.91 $x10^{-4}$ ± 1.69 $x10^{-5}$
B Power	4.95 ± 0.03	-	1.99 ± 0.01
χ^2	20.9	6.4	2.97

Table S4. Fitting parameters for SAXS data of 2NapFFD solutions with $CaCl_2$

Counterions	Li	Na	TBA
Model	Flexible cylinder + Cylinder	Flexible elliptical cylinder	Flexible cylinder + Power law
Background (cm^{-1})	0.005	0.039	0.0052
A Scale	0.00324 ± 1.28 $x10^{-5}$	0.002298 ± 7.38 $x10^{-6}$	0.0055 ± 7.99 $x10^{-6}$
A Length (Å)	>1000	>1000	>1000
A Kuhn Length (Å)	129 ± 0.3	134 ± 0.5	122 ± 0.4
A Radius (Å)	59.7 ± 0.1	29.1 ± 0.05	50.5 ± 0.03
A Axis ratio	-	2.33 ± 0.01	-
B Scale	0.00178 ± 1.39 $x10^{-5}$	-	3.51 $x10^{-5}$ ± 1.07 $x10^{-6}$
B Length (Å)	>1000	-	-
B Radius (Å)	48.5 ± 0.1	-	-
B Power	-	-	2.75 ± 0.01
χ^2	2.7	5.8	30.0

Table S5. Fitting parameters for SANS data of 2NapFFD.Na-with added LiCl

Eq of LiCl	2NapFFD.Na	2NapFFD.Na + 1 eq LiCl	2NapFFD.Na + 2 eq LiCl	2NapFFD.Na + 3 eq LiCl	2NapFFD.Na + 4 eq LiCl	2NapFFD.Na + 5 eq LiCl
Model	Cylinder + Power law	Cylinder + Hollow cylinder				
Background (cm^{-1})	0.011	0.019	$0.0197 \pm 5.73 \times 10^{-5}$	0.014	0.011	0.011
A Scale	$0.017 \pm 8.14 \times 10^{-5}$	0.21 ± 0.001	$0.0121 \pm 7.68 \times 10^{-5}$	0.12 ± 0.001	0.011 ± 0.0001	$0.008 \pm 9.2 \times 10^{-5}$
A Length (Å)	30.3 ± 0.3	>1000	>1000	>1000	>1000	>1000
A Radius (Å)	9.2 ± 0.04	46.6 ± 0.1	48.1 ± 0.1	48.4 ± 0.1	47.1 ± 0.07	46.6 ± 0.1
B Scale	$3.0 \times 10^{-6} \pm 2.9 \times 10^{-7}$	0.18 ± 0.001	$0.0133 \pm 7.67 \times 10^{-5}$	0.013 ± 0.001	0.012 ± 0.0001	$0.008 \pm 9.2 \times 10^{-5}$
B Power	2.59 ± 0.01	-	-	-	-	-
B Length (Å)	-	112 ± 1	>1000	>1000	>1000	>1000
B Radius (Å)	-	14.0 ± 0.07	11.2 ± 0.04	11.3 ± 0.05	11.3 ± 0.07	10.5 ± 0.05
B Thick-ness (Å)	-	20.1 ± 0.1	24.1 ± 0.1	23.9 ± 0.09	23.8 ± 0.1	25.2 ± 0.1
χ^2	2.27	30.28	13.7	12.6	12.1	15.9

Table S6. Fitting parameters for SANS data of 2NapFFD.Na-with added LiBr

Sample	2NapFFD.Na + 1 eq LiBr	2NapFFD.Na + 5 eq LiBr
Model	Cylinder + Hollow cylinder	
Background (cm^{-1})	$0.00845 \pm 2.91 \times 10^{-5}$	$0.00862 \pm 2.83 \times 10^{-5}$
A Scale	$0.00410 \pm 1.89 \times 10^{-5}$	$0.00595 \pm 4.01 \times 10^{-5}$
A Length (Å)	>1000	>1000
A Radius (Å)	46.1 ± 0.1	47.2 ± 0.06
B Scale	$0.00365 \pm 2.05 \times 10^{-5}$	$0.00556 \pm 4.12 \times 10^{-5}$
B Length (Å)	117 ± 1	>1000
B Radius (Å)	14.7 ± 0.07	11.9 ± 0.05
B Thickness (Å)	18.9 ± 0.1	22.5 ± 0.1
χ^2	11.3	17.5

Table S7. Fitting parameters for SANS data of 2NapFFD.Na-with added NaCl and KCl

Sample	2NapFFD.Na + 1 eq NaCl	2NapFFD.Na + 5 eq NaCl	2NapFFD.Na + 1 eq KCl	2NapFFD.Na + 5 eq KCl
Model	Cylinder + Power law			
Background (cm^{-1})	$0.0116 \pm 3.52 \times 10^{-5}$	$0.00957 \pm 3.23 \times 10^{-5}$	$0.00968 \pm 3.45 \times 10^{-5}$	$0.00745 \pm 3.18 \times 10^{-5}$
A Scale	$0.00700 \pm 2.84 \times 10^{-5}$	$0.00789 \pm 2.11 \times 10^{-5}$	$0.00680 \pm 2.72 \times 10^{-5}$	$0.00747 \pm 2.03 \times 10^{-5}$
A Length (Å)	32.2 ± 0.2	36.7 ± 0.2	32.6 ± 0.2	37.6 ± 0.2
A Radius (Å)	10.4 ± 0.04	12.0 ± 0.03	10.5 ± 0.04	12.4 ± 0.03
B Scale	$1.50 \times 10^{-6} \pm 1.73 \times 10^{-7}$	$5.48 \times 10^{-6} \pm 4.40 \times 10^{-7}$	$1.20 \times 10^{-6} \pm 1.44 \times 10^{-7}$	$5.66 \times 10^{-6} \pm 6.53 \times 10^{-7}$
B Power	2.60 ± 0.02	2.45 ± 0.01	2.63 ± 0.02	2.36 ± 0.02
χ^2	2.04	3.06	2.47	2.52

Table S8. Fitting parameters for SAXS data of 2ThNapFFD.Li solution

	2ThNapFFD.Li
Model	Cylinder + Hollow cylinder
Background (cm^{-1})	0.00283 ± 1.02 $x10^{-4}$
A Scale	0.00292 ± 2.86 $x10^{-6}$
A Length (Å)	>1000
A Radius (Å)	56.2 ± 0.1
B Scale	0.00199 ± 4.60 $x10^{-6}$
B Length (Å)	>1000
B Radius (Å)	11.1 ± 0.0
B Thickness (Å)	20.6 ± 0.1
χ^2	29.8

Table S9. Fitting parameters for SAXS data of 2ThNapFFD salts with counterions other than Li

Counterions	Na	K	Rb	Cs	TBA	BTMA
Model	Cylinder + Power law					
Background (cm^{-1})	0.004	0.005	0.005	0.01	0.003	0.0025
A Scale	0.000911 ± 1.84 $x10^{-5}$	0.000968 ± 1.99 $x10^{-5}$	0.0019 ± 2.87 $x10^{-5}$	0.0025 ± 3.17 $x10^{-5}$	0.001154 ± 7.43 $x10^{-5}$	0.001121 ± 7.42 $x10^{-5}$
A Length (Å)	725 ± 14	139 ± 4	777 ± 94	741 ± 72	29.4 ± 6.8	29.4 ± 14.8
A Radius (Å)	17.4 ± 0.2	17.5 ± 0.2	14.5 ± 0.1	13.9 ± 0.1	17.0 ± 0.8	17.0 ± 0.6
B Scale	1.38 $x10^{-8}$ ± 2.82 $x10^{-10}$	3.06 $x10^{-7}$ ± 6.75 $x10^{-9}$	3.89 $x10^{-7}$ ± 7.24 $x10^{-9}$	8.10 $x10^{-7}$ ± 9.80 $x10^{-9}$	8.82 $x10^{-8}$ ± 2.11 $x10^{-9}$	9.05 $x10^{-8}$ ± 2.25 $x10^{-9}$
B Power	3.65 ± 0.03	3.50 ± 0.00	3.47 ± 0.003	3.42 ± 0.002	3.67 ± 0.004	3.66 ± 0.004
χ^2	0.5	2.71	3.13	8.51	1.95	1.86

Table S10. Fitting parameters for SAXS data of 1ThNapFFD.Li solution

	1ThNapFFD.Li
Model	Elliptical Cylinder + Power law
Background (cm^{-1})	0.004
A Scale	$0.00178 \pm 2.20 \times 10^{-6}$
A Length (Å)	322 ± 3
A Radius (Å)	45.2 ± 0.04
A Axis ratio	2.25 ± 0.003
B Scale	$0.00118 \pm 1.04 \times 10^{-5}$
B power	1.9 ± 0.0017
χ^2	26.24

Table S11. Fitting parameters for SAXS data of 1ThNapFFD salts with counterions other than Li

Counterions	Na	K	Rb	Cs	TBA	BTMA
Model	Cylinder + Power law					
Background (cm^{-1})	0.004	0.005	0.006	0.009	0.0025	0.003
A Scale	$0.00134 \pm 2.04 \times 10^{-7}$	$0.00101 \pm 4.99 \times 10^{-6}$	$0.00245 \pm 2.68 \times 10^{-5}$	$0.00262 \pm 2.40 \times 10^{-5}$	$0.001324 \pm 7.26 \times 10^{-5}$	$0.00128 \pm 7.55 \times 10^{-5}$
A Length (Å)	185 ± 5	277 ± 4	765 ± 67	771 ± 58	29.1 ± 2.7	29.2 ± 2.8
A Radius (Å)	17.1 ± 0.16	37.7 ± 0.10	14.9 ± 0.09	15.6 ± 0.1	17.0 ± 6.9	16.9 ± 8.6
B Scale	$2.00 \times 10^{-7} \pm 1.54 \times 10^{-8}$	$1.88 \times 10^{-5} \pm 3.27 \times 10^{-7}$	$5.23 \times 10^{-7} \pm 9.0 \times 10^{-9}$	$7.55 \times 10^{-7} \pm 1.04 \times 10^{-8}$	$1.09 \times 10^{-7} \pm 8.44 \times 10^{-9}$	$8.64 \times 10^{-8} \pm 8.91 \times 10^{-9}$
B Power	3.37 ± 0.01	2.83 ± 0.003	3.43 ± 0.003	3.40 ± 0.002	3.39 ± 0.014	3.38 ± 0.019
χ^2	0.67	8.05	3.93	7.11	0.63	0.59

Table S12. Fitting parameters for SANS data of 2ThNapFFD.Na-with added LiCl

Eq of LiCl	2ThNapFFD. Na	2ThNapFFD.Na + 1 eq LiCl	2ThNapFFD. Na + 2 eq LiCl	2ThNapFFD. Na + 3 eq LiCl	2ThNapFFD. Na + 4 eq LiCl	2ThNapFFD. Na + 5 eq LiCl
Model	Cylinder + Power law	Cylinder + Hollow cylinder				
Background (cm^{-1})	0.011 ± 3.3 $x10^{-5}$	0.00924 ± 2.87 $x10^{-5}$	0.00735 ± 2.84 $x10^{-5}$	0.0068 ± 2.86 $x10^{-5}$	0.0076 ± 2.87 $x10^{-5}$	0.0096 ± 2.9 $x10^{-5}$
A Scale	0.0074 ± 2.37 $x10^{-5}$	0.00369 ± 2.39 $x10^{-5}$	0.00521 ± 2.14 $x10^{-5}$	0.00611 ± 2.52 $x10^{-5}$	0.0057 ± 2.33 $x10^{-5}$	0.006 ± 2.4 $x10^{-5}$
A Length (Å)	69.2 ± 0.5	>1000	>1000	>1000	>1000	>1000
A Radius (Å)	10.7 ± 0.02	47.4± 0.1	49.6 ± 0.1	48.1 ± 0.1	49.7 ± 0.1	49.1 ± 0.1
B Scale	4.7 $x10^{-6}$ ± 1.9 $x10^{-8}$	0.0068 ± 2.58 $x10^{-5}$	0.00695 ± 2.36 $x10^{-5}$	0.00675 ± 2.60 $x10^{-5}$	0.0073 ± 2.46 $x10^{-5}$	0.0073 ± 2.56 $x10^{-5}$
B Power	2.59 ± 0.01	-	-	-	-	-
B Length (Å)	-	121 ± 1	128 ± 1	130 ± 1	137 ± 1	129 ± 1
B Radius (Å)	-	13.7 ± 0.04	12.8 ± 0.04	12.9 ± 0.05	12.5 ± 0.03	12.7 ± 0.03
B Thick-ness (Å)	-	21.3 ± 0.1	22.1 ± 0.1	21.3 ± 0.1	22.1 ± 0.1	22.0 ± 0.1
χ^2	7.06	32.8	14.2	19.6	20.3	25.1

Table S13. Fitting parameters for SANS data of 1ThNapFFD.Na-with added LiCl

Sample	1ThNapFFD. Na	1ThNapFFD.Na + 1 eq LiCl	1ThNapFFD. Na + 2 eq LiCl	1ThNapFFD. Na + 3 eq LiCl	1ThNapFFD. Na + 4 eq LiCl	1ThNapFFD. Na + 5 eq LiCl
Model	Cylinder + Power law	Elliptical cylinder + Power law				
Background (cm^{-1})	0.0148 ± 3.44 $x10^{-5}$	0.0083 ± 3.12 $x10^{-5}$	0.00872 ± 2.94 $x10^{-5}$	0.0065 ± 3.32 $x10^{-5}$	0.0173 ± 6.54 $x10^{-5}$	0.0119 ± 6.54 $x10^{-5}$
A Scale	0.0146 ± 3.77 $x10^{-5}$	0.00995 ± 1.97 $x10^{-5}$	0.0102 ± 1.40 $x10^{-5}$	0.0101 ± 1.97 $x10^{-5}$	0.0194 ± 3.63 $x10^{-5}$	0.0187 ± 3.73 $x10^{-5}$
A Length (Å)	38.2 ± 0.2	>1000	>1000	133 ± 1	117 ± 1	128 ± 1
A Radius (Å)	10.9 ± 0.02	10.6 ± 0.03	13.8 ± 0.02	17.2 ± 0.03	18.4 ± 0.03	17.1 ± 0.03
A Axis ratio	-	3.07 ± 0.01	2.34 ± 0.01	2.02 ± 0.01	1.96 ± 0.01	2.02 ± 0.01
B Scale	6.19$x10^{-6}$ ± 8.17 $x10^{-8}$	5.42 $x10^{-6}$ ± 1.26 $x10^{-7}$	3.52 $x10^{-6}$ ± 9.12 $x10^{-8}$	7.60 $x10^{-5}$ ± 1.39 $x10^{-6}$	1.53 $x10^{-4}$ ± 2.48 $x10^{-6}$	0.000145 ± 2.65 $x10^{-6}$
B Power	2.81 ± 0.00	2.83 ± 0.04	2.89 ± 0.04	2.40 ± 0.03	2.41 ± 0.02	2.40 ± 0.03
χ^2	28.0	30.28	29.5	9.83	12.1	8.59

Table S14. Fitting parameters for SAXS data of 2NapFD solutions

Counterions	Li	Na	TBA
Model	Cylinder + Power law		
Background (cm^{-1})	0.004	0.009	0.01
A Scale	0.00464 ± 3.45 $x10^{-5}$	0.00234 ± 2.90 $x10^{-5}$	0.00051 ± 0.00018
A Length (Å)	62.2 ± 0.2	36.7 ± 1.0	32.9 ± 0.1
A Radius (Å)	42.7 ± 0.1	9.6 ± 0.9	9.9 ± 0.0
B Scale	3.26 $x10^{-6}$ ± 4.27 $x10^{-8}$	1.33 $x10^{-6}$ ± 9.65 $x10^{-8}$	1.37 $x10^{-8}$ ± 1.54 $x10^{-9}$
B Power	3.11 ± 0.00	2.86 ± 0.01	3.72 ± 0.20
χ^2	4.45	0.40	0.38

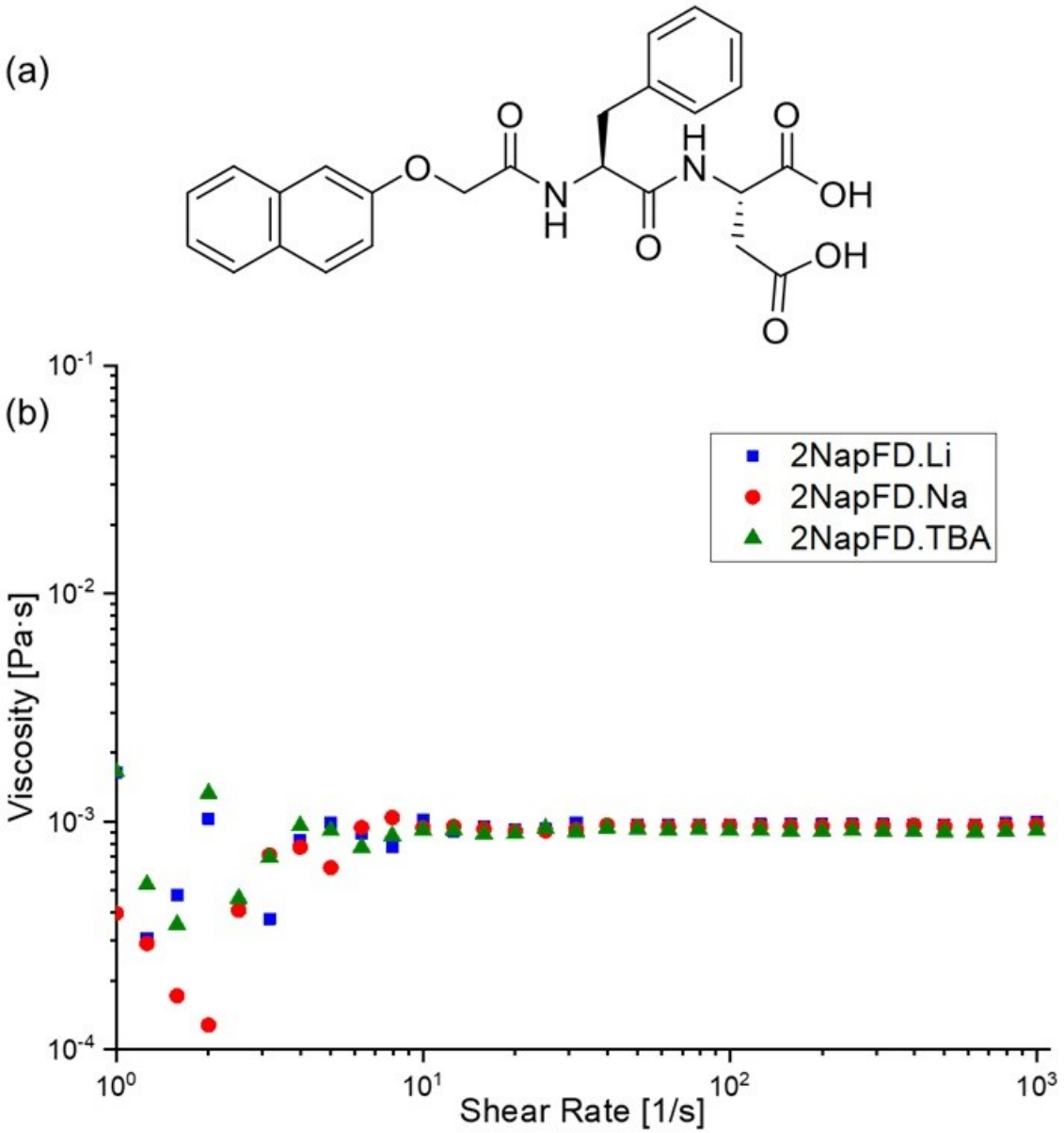


Figure S24: (a) Chemical structure of 2NapFD. (b) Viscosity profiles of its Li^+, Na^+, and TBA^+ salts (20 mg/mL, pH 10.5) measured as a function of shear rate (bottom). All samples exhibit low viscosities comparable to water, indicating the absence of significant self-assembly.

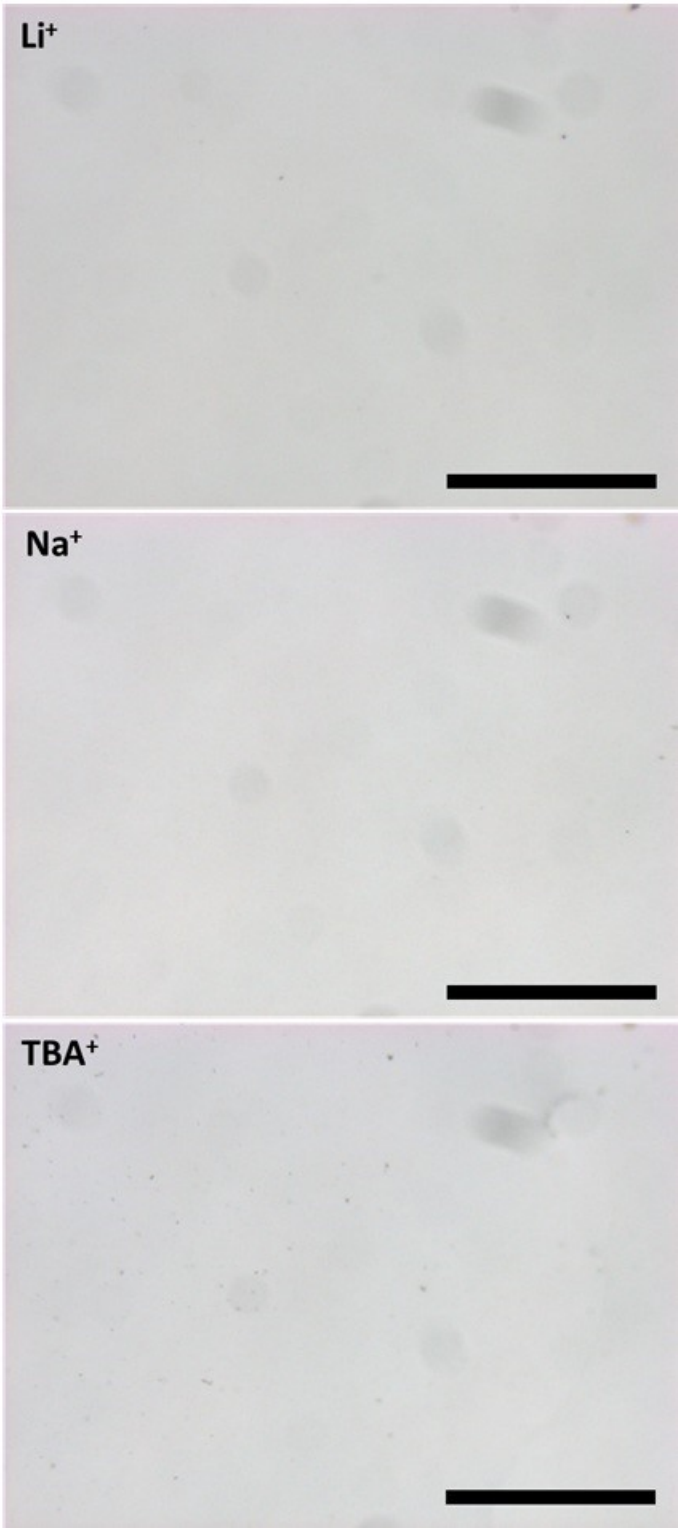


Figure S25: Brightfield optical micrographs of 2NapFD solutions prepared with Li^+, Na^+, and TBA^+ counterions (20 mg/mL, pH 10.5). The polarised images of all the solutions appeared completely black. Scale bars: 500 μm.

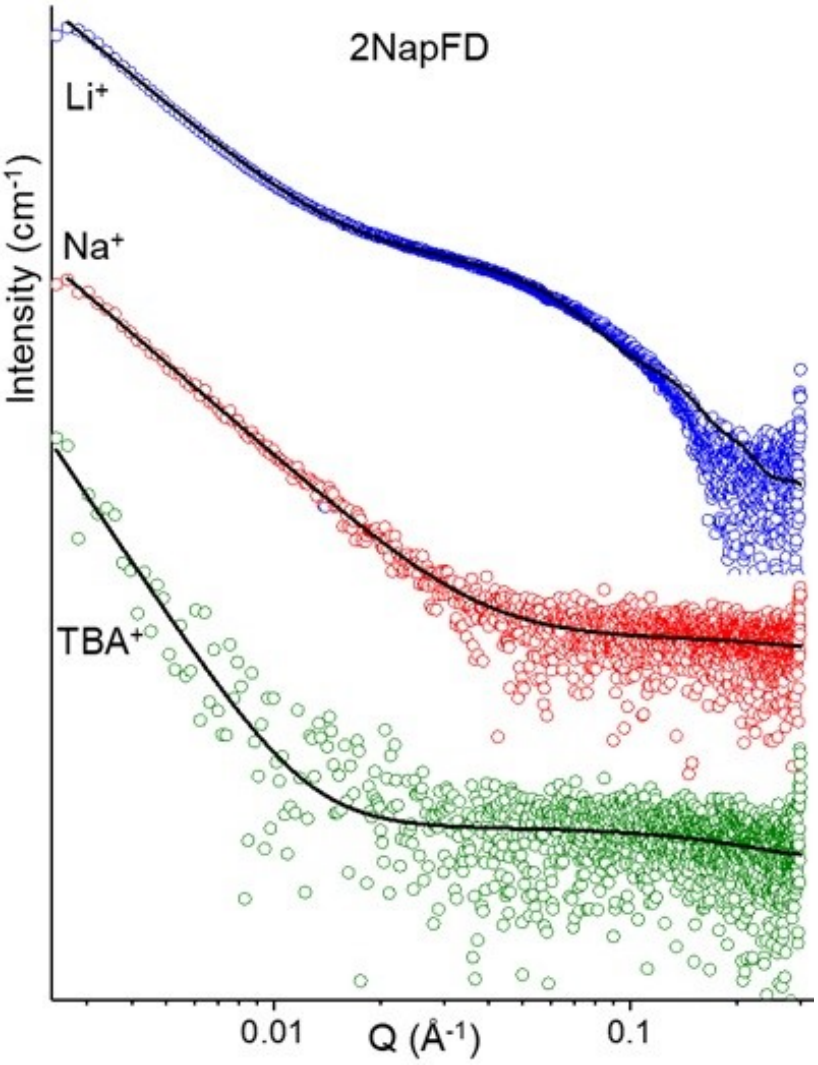


Figure S26: SAXS profiles of 2NapFD prepared with different counterions (Li^+, Na^+, and TBA^+) at pH 10.5 and 20 mg/mL. Symbols show the experimental data and solid lines show the best fits (power law + cylinder model), indicating only short, weakly aggregated structures across all three salts.

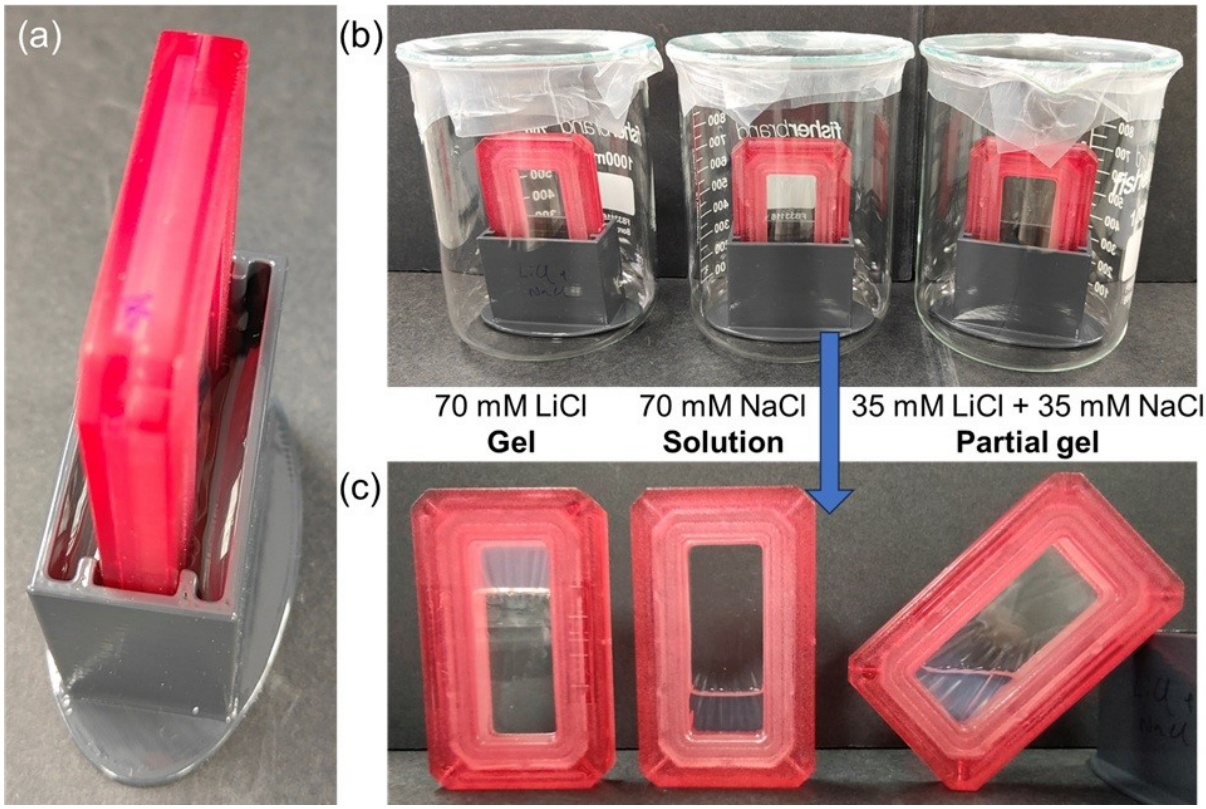


Figure S27: Dialysis setup used for ICP-OES quantification of ion uptake. (a) Custom 3D-printed cassette holder to minimize NaCl/LiCl dialysate volume. (b) Dialysis set up using 70 mM LiCl, 70 mM NaCl, or 35 mM LiCl + 35 mM NaCl as the external solutions. (c) Dialysis cassettes after dialysis, showing gel formation for LiCl, no gel for NaCl, and partial gelation for the mixed-salt condition.