Supplemental Information for:

Bridging the Crystal and Solution Structure of a Series of Lipid-Inspired Ionic Liquids

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	2	3	4
Crystal data			
Chemical formula	$Br \cdot C_{21}H_{41}N_2$	$I \cdot C_{21}H_{41}N_2$	$C_{21}H_{41}N_2 \cdot C_2F_6NO_4S_2$
M_r	401.47	448.46	601.71
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$
Temperature (K)	150	150	150
a, b, c (Å)	6.715 (3), 7.437 (2), 24.396 (9)	27.660 (9), 9.9680 (19), 8.2860 (16)	7.0531 (2), 15.7762 (5), 27.1070 (9)
α(°)	86.48 (2),	90	96.4858 (18)
β(°)	82.188 (17)	91.613 (12)	95.9509 (17)
γ(°)	68.301 (12)	90	98.1327 (17)
V (Å^3)	1121.5 (7)	2283.7 (10)	2944.75 (16)
Z	2	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	2.51	11.03	2.28
Crystal size (mm)	0.34 × 0.32 × 0.14	0.15 × 0.09 × 0.001	0.19 × 0.16 × 0.05
Data collection			
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0981 before and 0.0621 after correction. The Ratio of minimum to maximum transmission is 0.5417. The λ/2 correction factor is not present.	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D. (2015). J. Appl. Cryst. 48, 3-10.	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.179, 0.330	0.044, 0.169	0.595, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9127, 4516, 4170	15434, 15434, 11213	28387, 12039, 9026
R_{int}	0.046	0.104	0.052
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.638	0.612	0.638
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.063, 0.169, 1.20	0.097, 0.297, 1.11	0.089, 0.261, 1.05
No. of reflections	4516	15434	12039
No. of parameters	220	223	1385
No. of restraints	-	-	2748
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.09, −0.60	3.26, −1.66	0.44, −0.34

Table S1. Experimental details for the crystallographic studies.

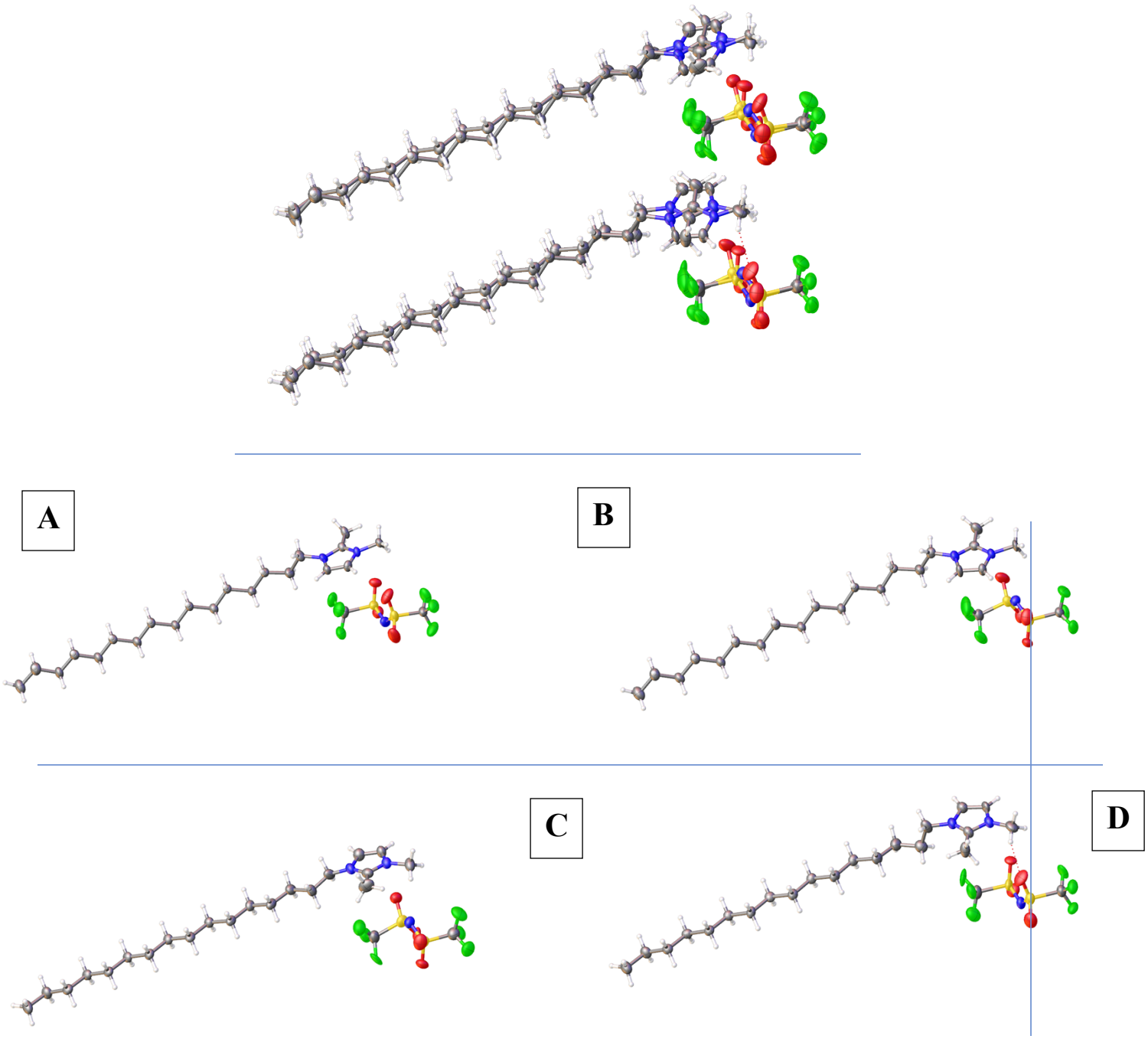

Figure S1. (top) The asymmetric unit of compound 4 shown with disorder. (bottom) The individual cation/anion pairs in the asymmetric unit.

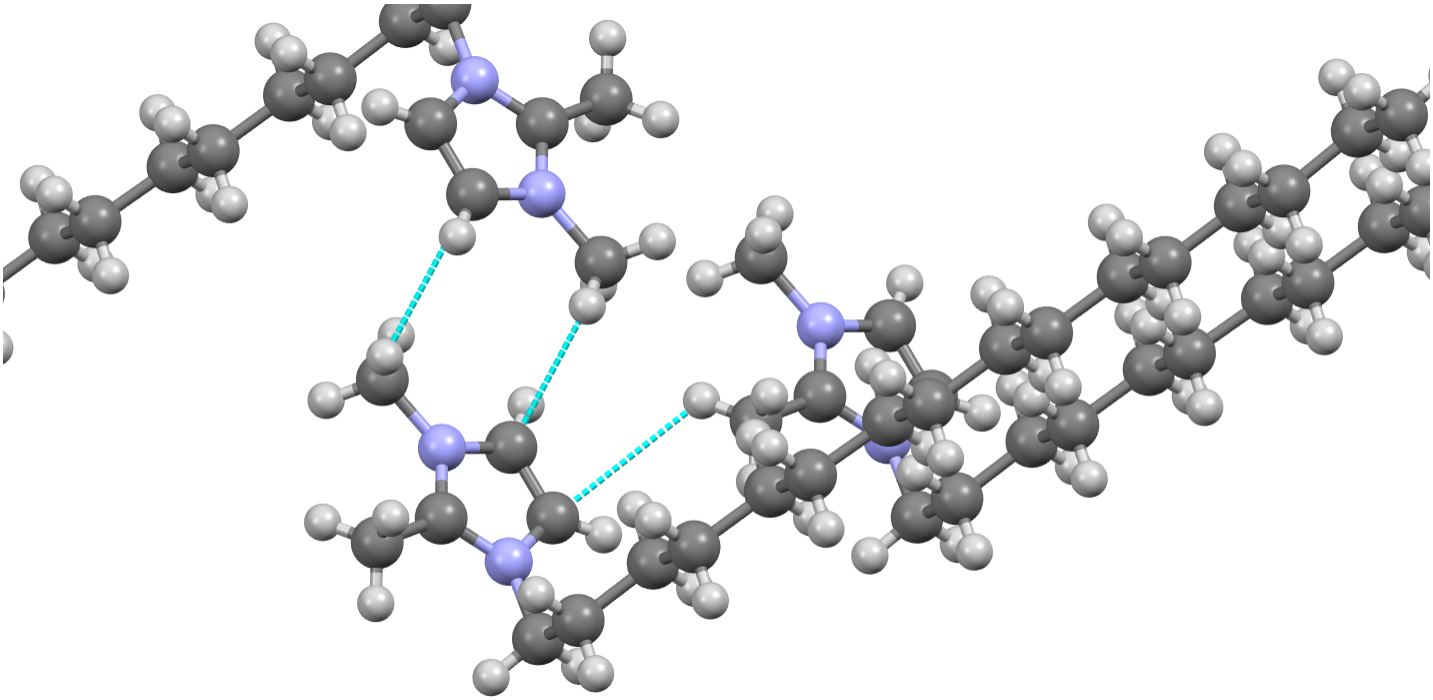

Figure S2. Depiction of the H···C|C···H interactions in **2**. Image is zoomed in to show only the heterocycle. The cutoff for interactions was set at the sum of the van der Waal radius + 0.2 Å. Longer interactions do also exist.

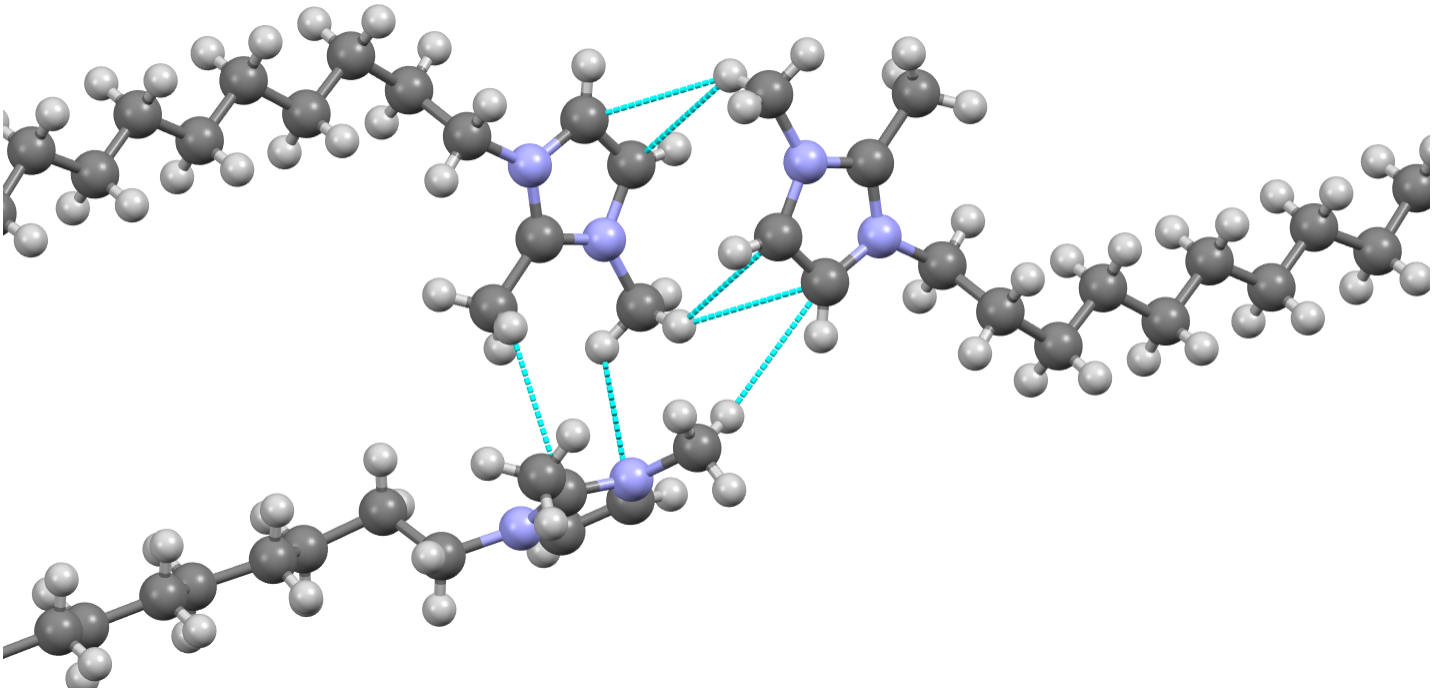

Figure S3. Depiction of the H···C|C···H interactions in **3**. Image is zoomed in to show only the heterocycle. The cutoff for interactions was set at the sum of the van der Waal radius + 0.2 Å. Longer interactions do also exist.

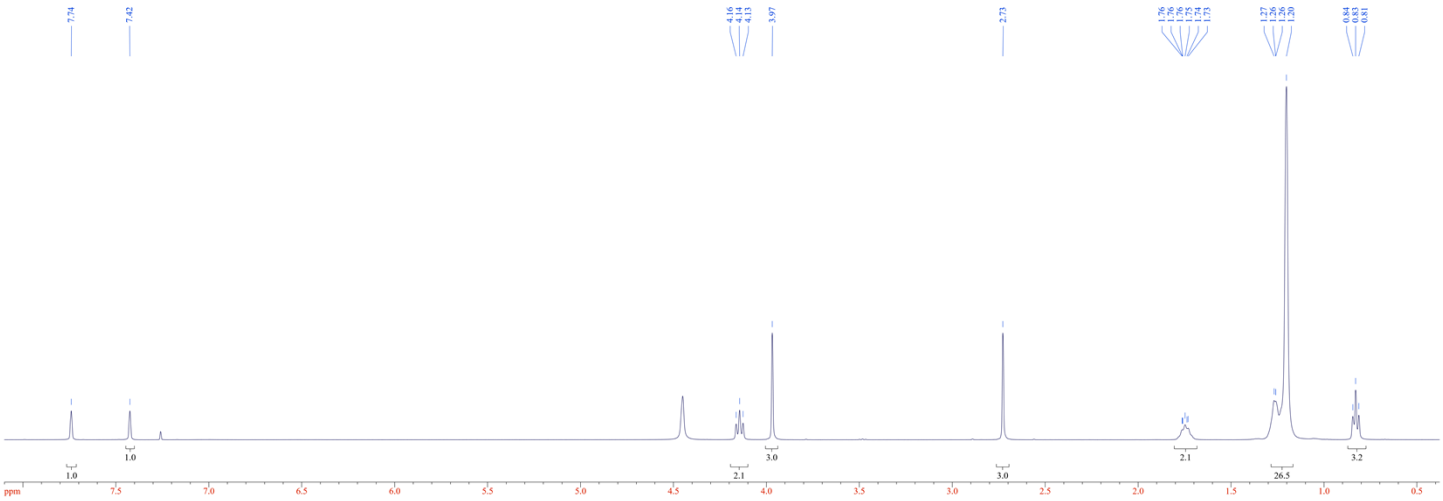

Figure S4. 1H NMR of Compound 1.

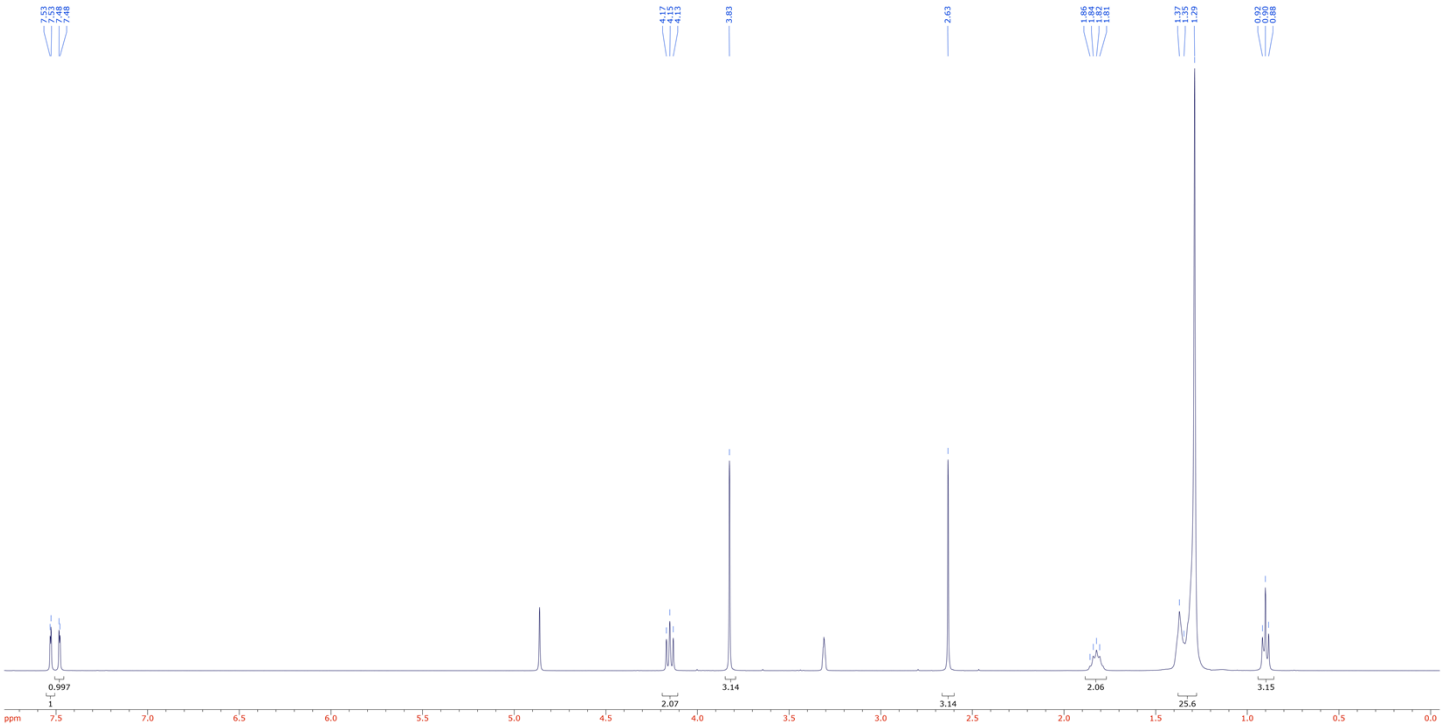

Figure S5. 1H NMR of Compound 2.

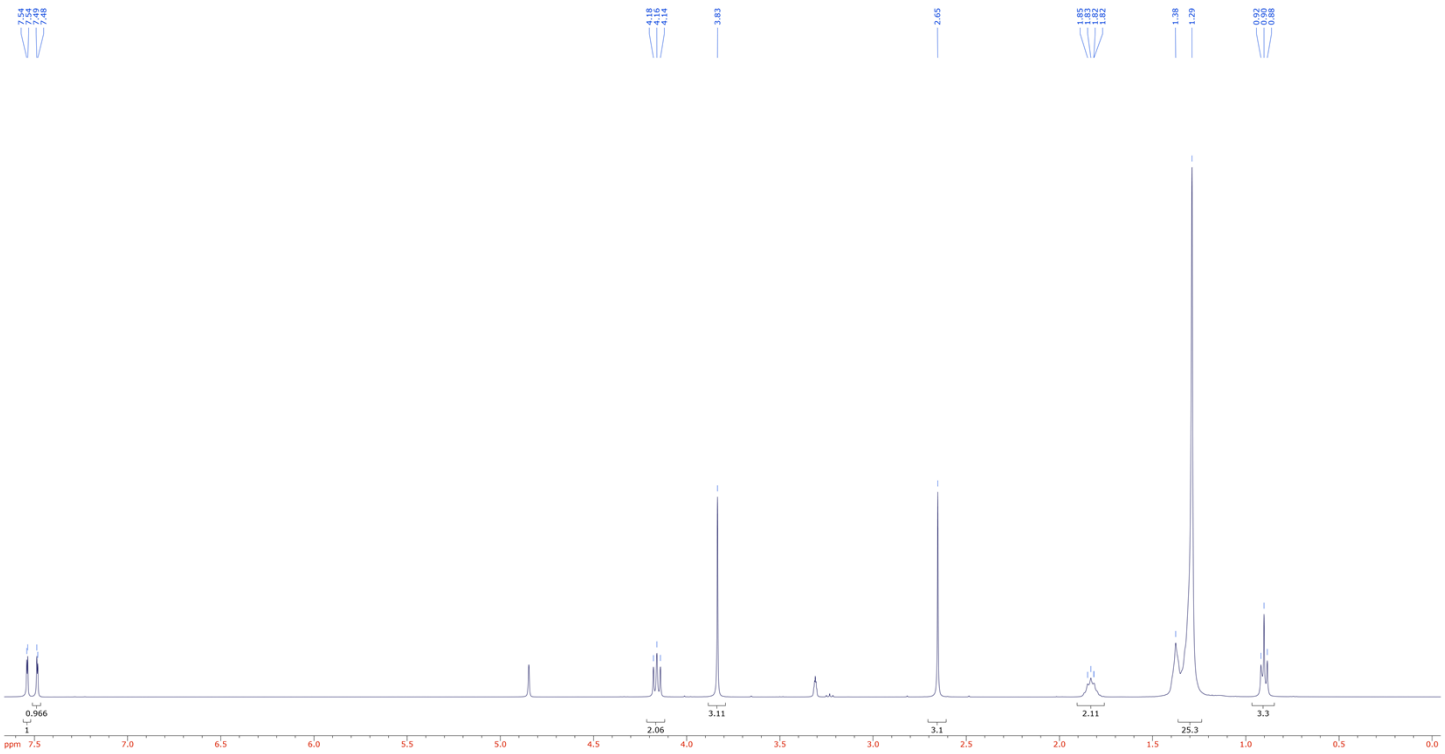

Figure S6. 1H NMR of Compound 3.

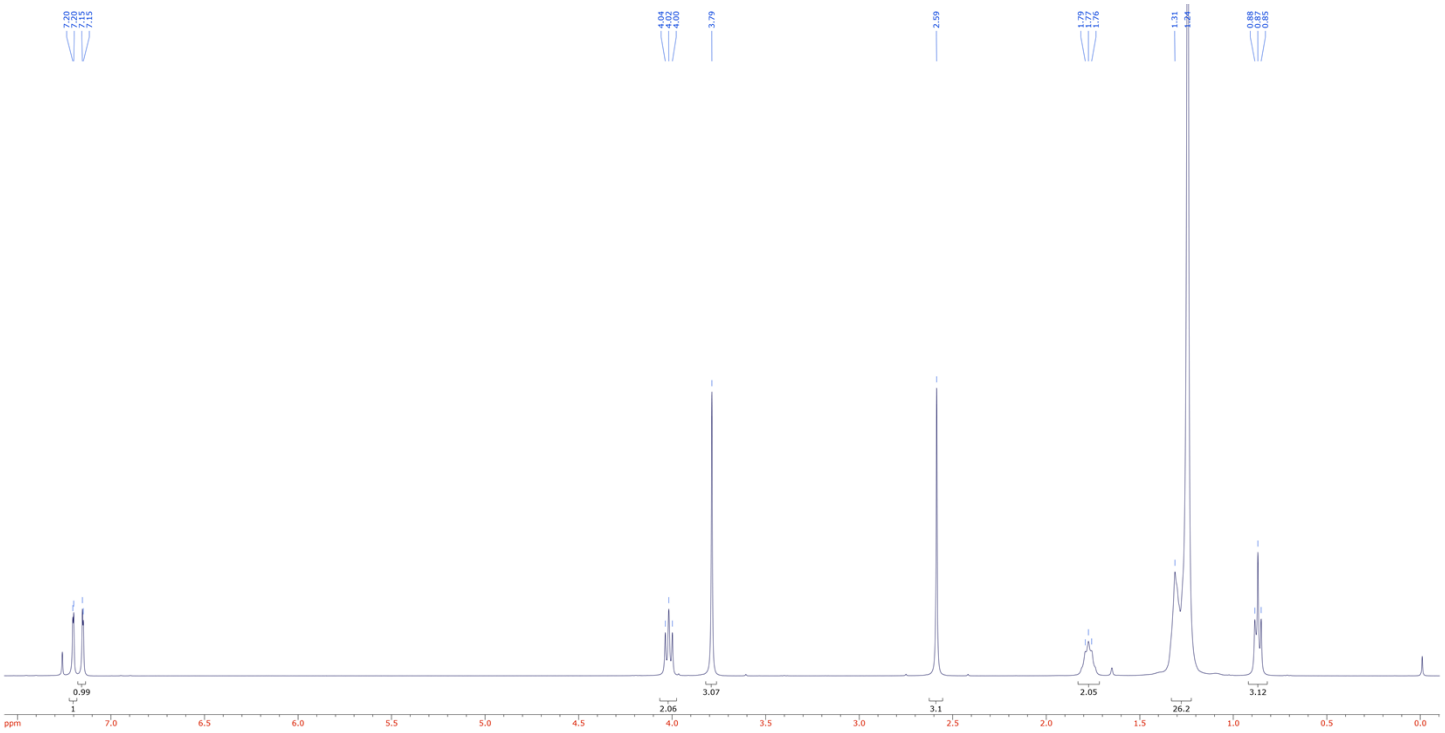

Figure S7. 1H NMR of Compound 4.

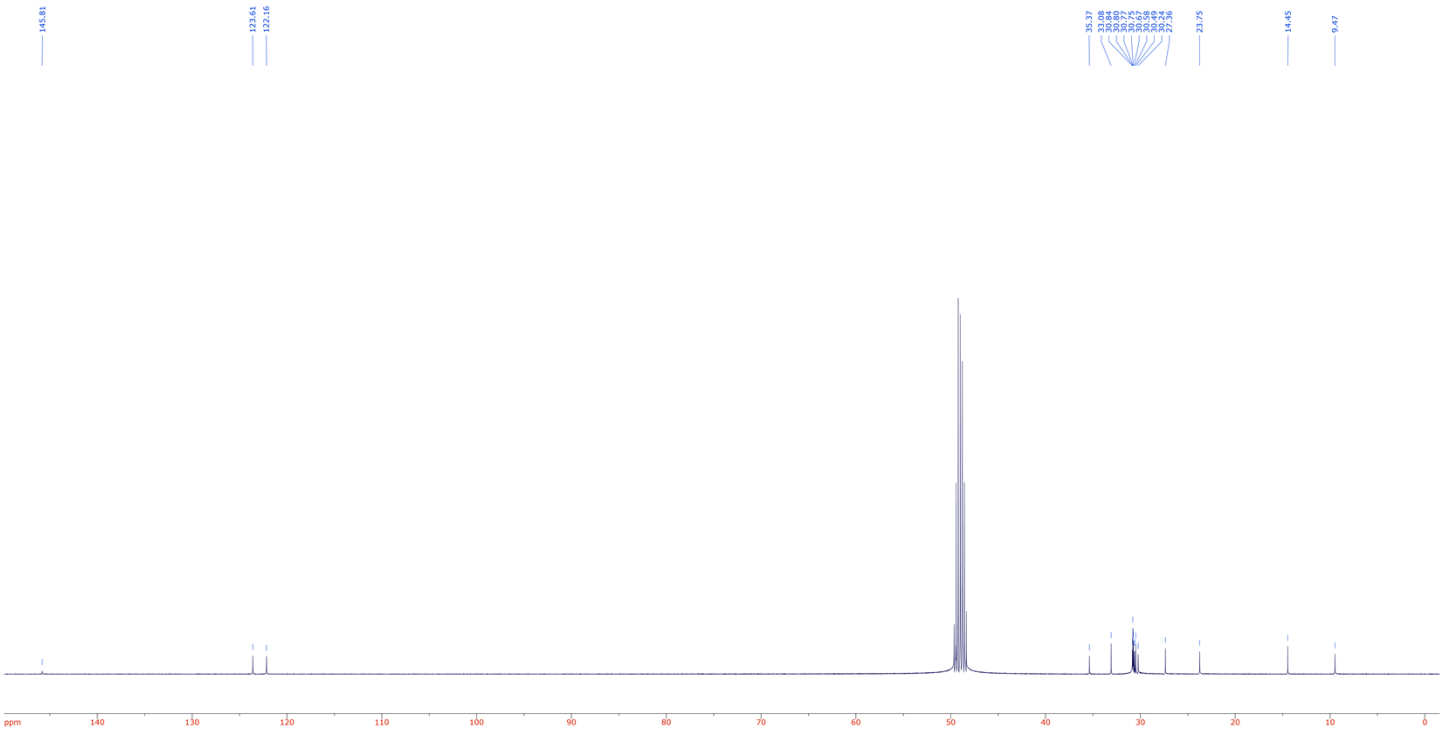

Figure S8. 13C NMR of Compound 1.

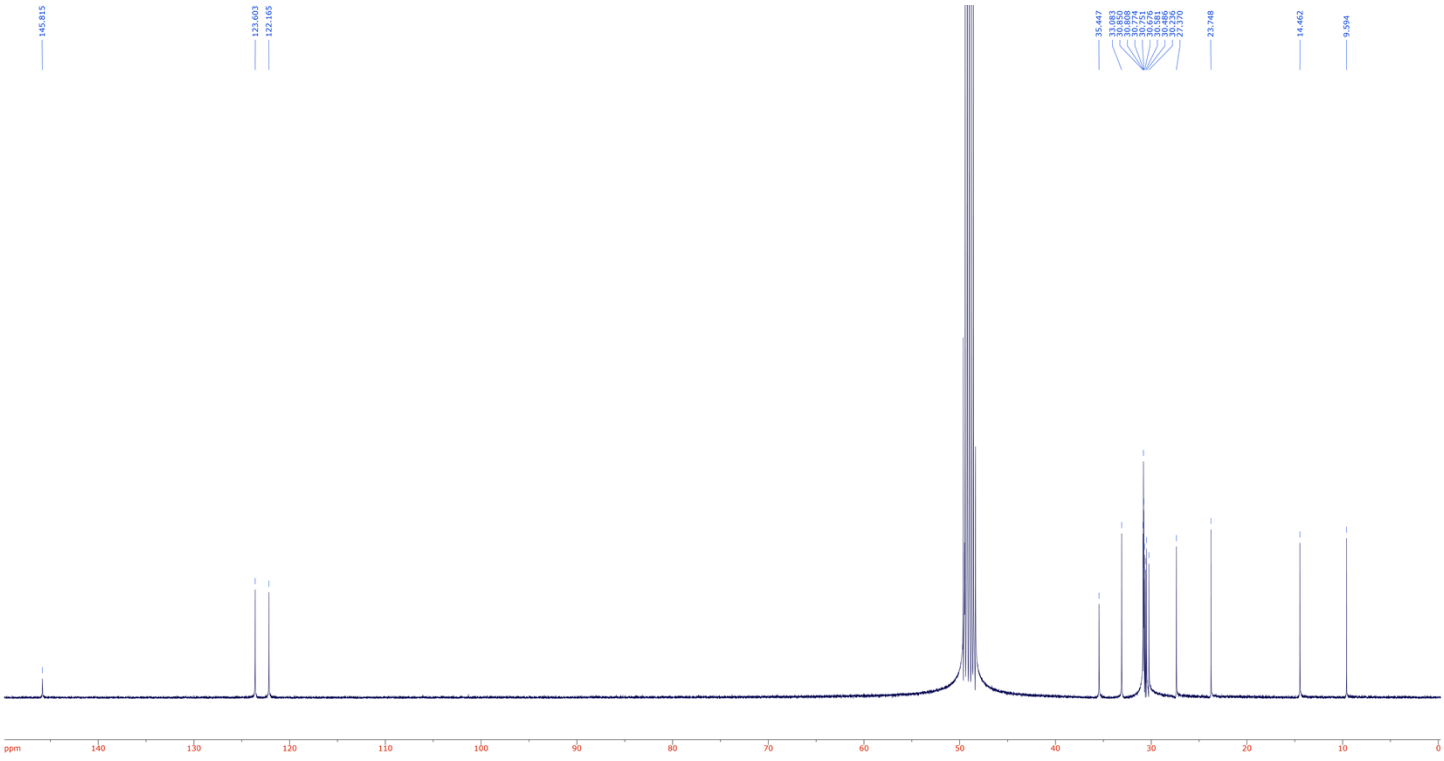

Figure S9. 13C NMR of Compound 2.

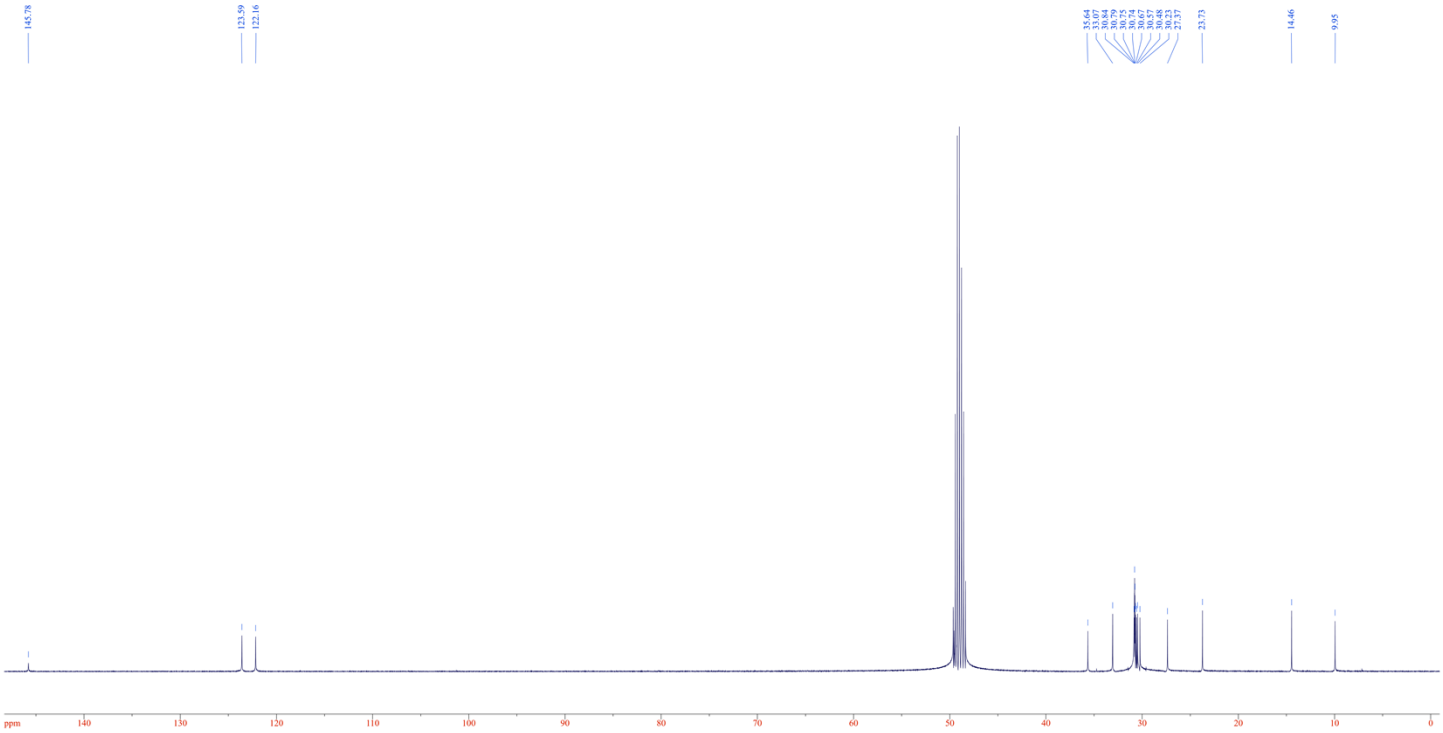

Figure S10. 13C NMR of Compound 3.

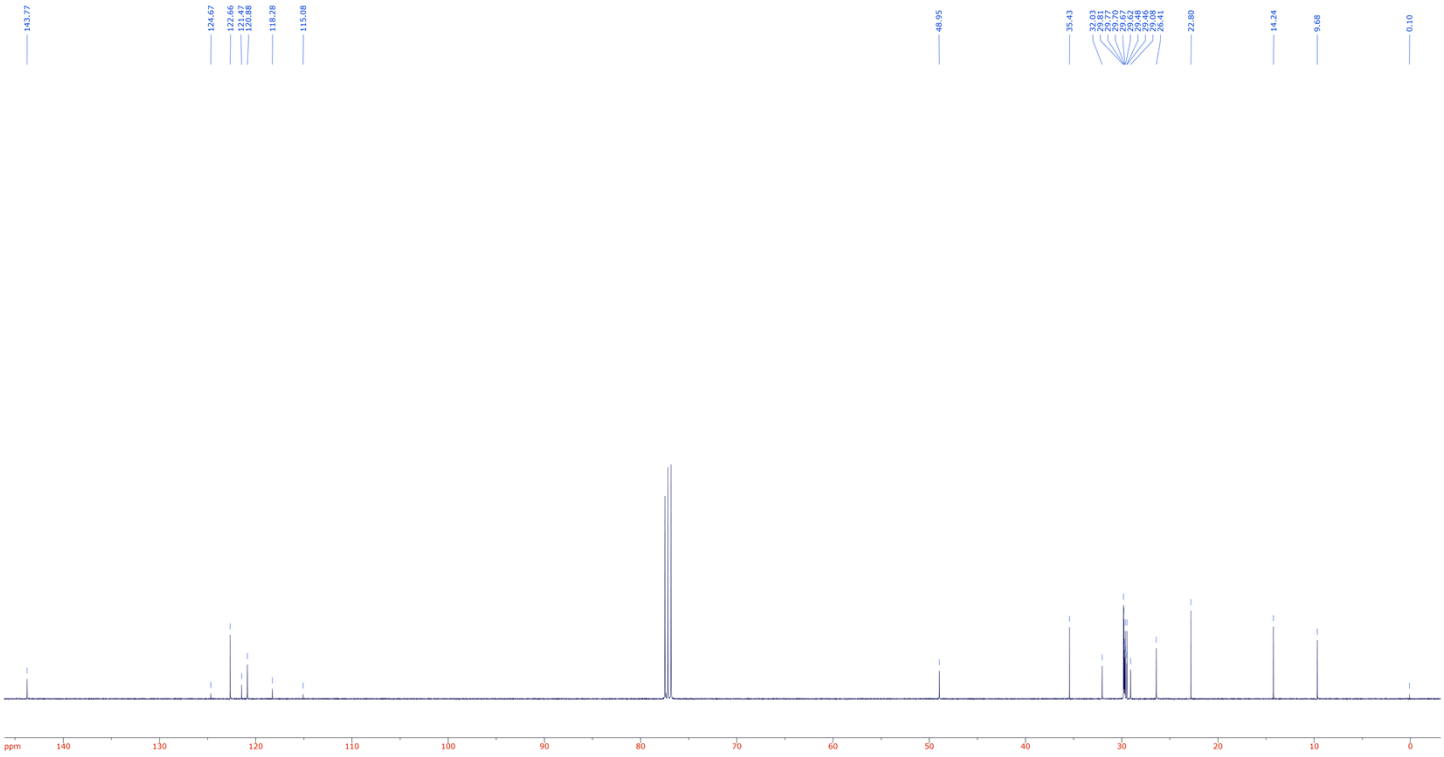

Figure S11. 13C NMR of Compound 4.

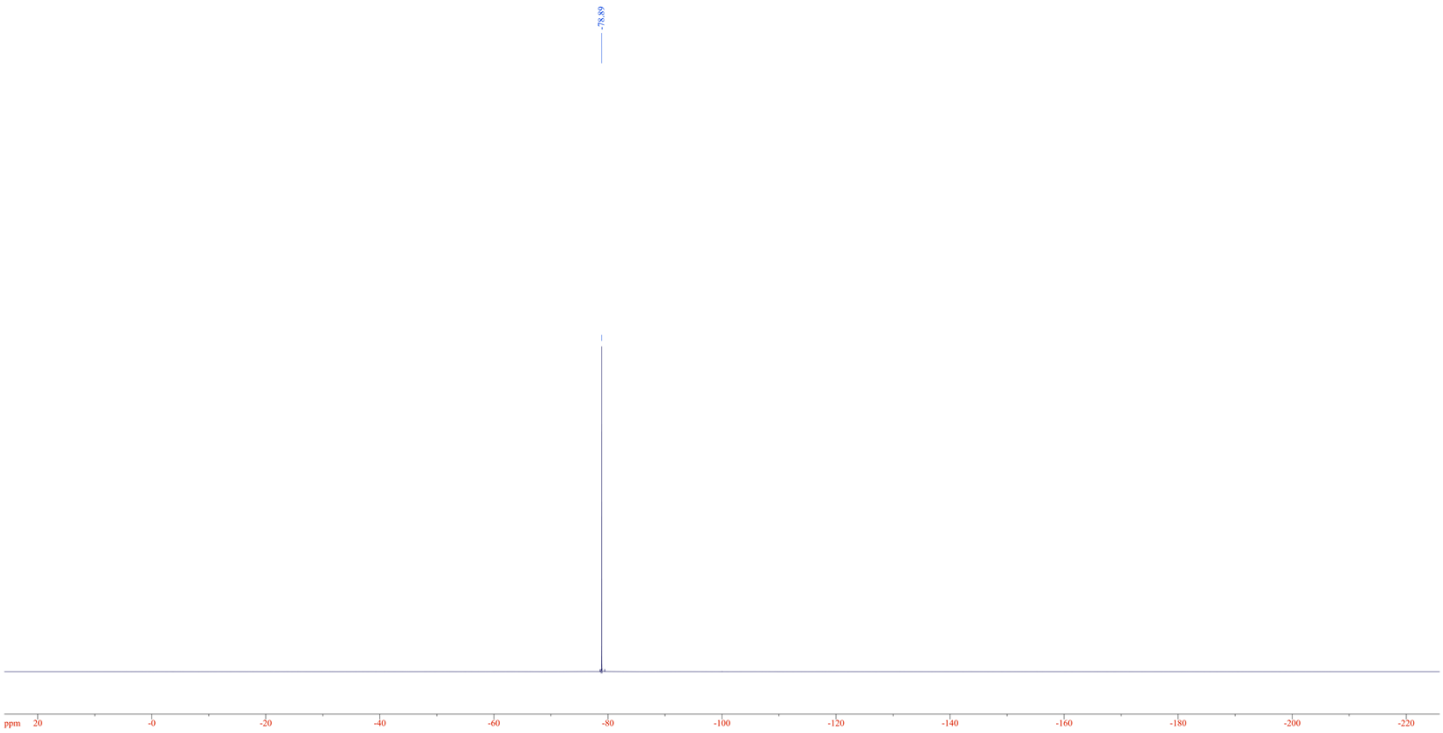

Figure S12. 19F NMR of Compound 4.