

Supplementary Materials

2-(2,6-Diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate

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List of content:

1. NMR ¹ H-spectra of compound 4	S2-S3
2. NMR ¹³ C-spectra of compound 4	S4-S5
3. NMR ¹ H-spectra of compound 2	S6-S7
4. NMR ¹³ C-spectra of compound 2	S8-S10
5. NMR 2D spectra – COSY, HSQC, HMBS of compound 2	S11-S12
6. NMR ¹ H and ¹³ C-spectra of compound 1 in DMSO	S13-S17
7. NMR 2D spectra – COSY, HSQC, HMBS of compound 1 in DMSO	S18-S19
8. NMR ¹ H and ¹³ C-spectra of compound 1 in metanol	S20-S24
9. NMR 2D spectra – COSY, HSQC, HMBS of compound 1 in metanol	S25-S26
10. UV, fluorescent and IR spectra of compound 1 in (a) MeOH and (b) MeCN.	S26-S28

NMR ^1H -spectra of compound **4**

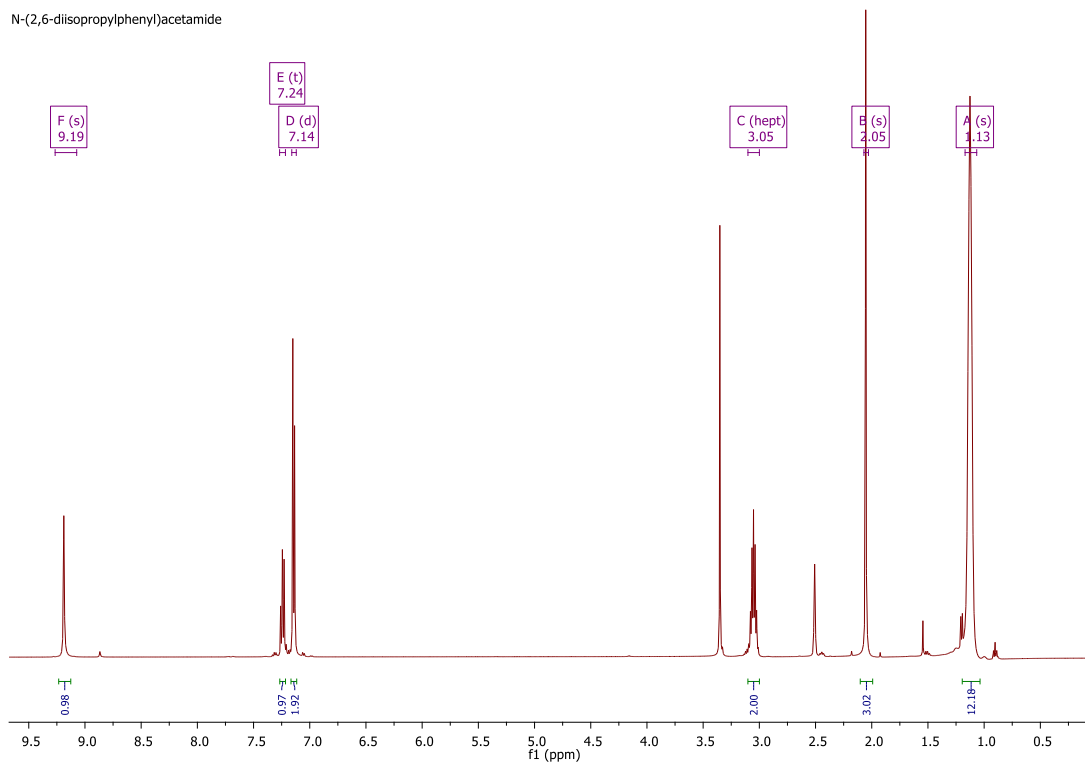


Figure S1. ^1H -NMR spectrum of N-(2,6-diisopropylphenyl)acetamide **4** in DMSO.

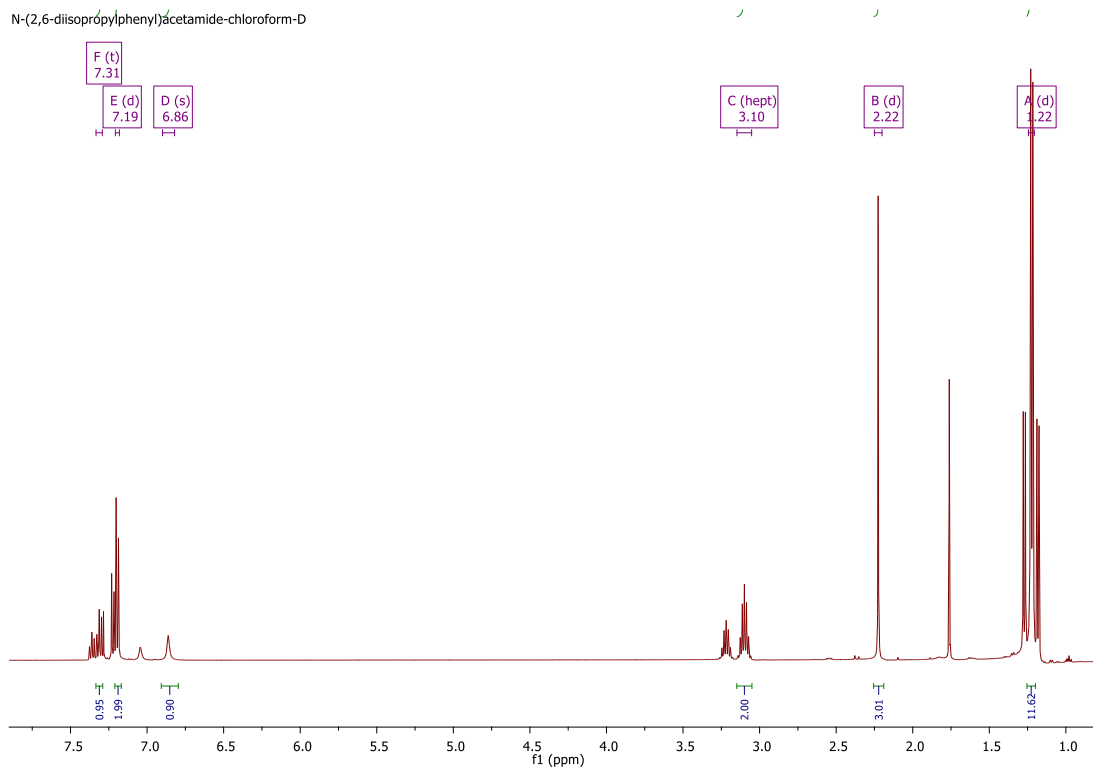


Figure S2. ^1H -NMR spectrum of N-(2,6-diisopropylphenyl)acetamide **4** in CDCl_3 . Only the signals of the major form are integrated and marked.

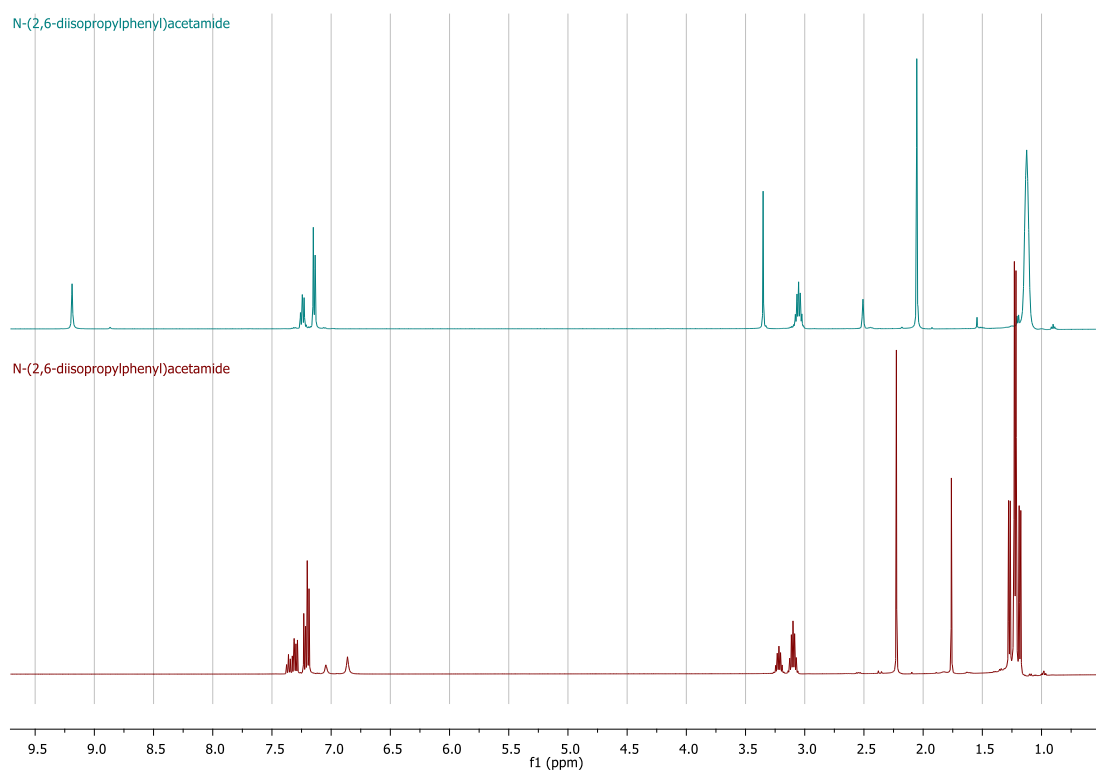


Figure S3. Comparison between ¹H-NMR spectra of N-(2,6-diisopropylphenyl)acetamide **4** in deuterated DMSO (blue coloured) and CDCl₃ (red coloured).

NMR ^{13}C -spectra of compound **4**

N-(2,6-diisopropylphenyl)acetamide-DMSO-d₆-DEPT-135

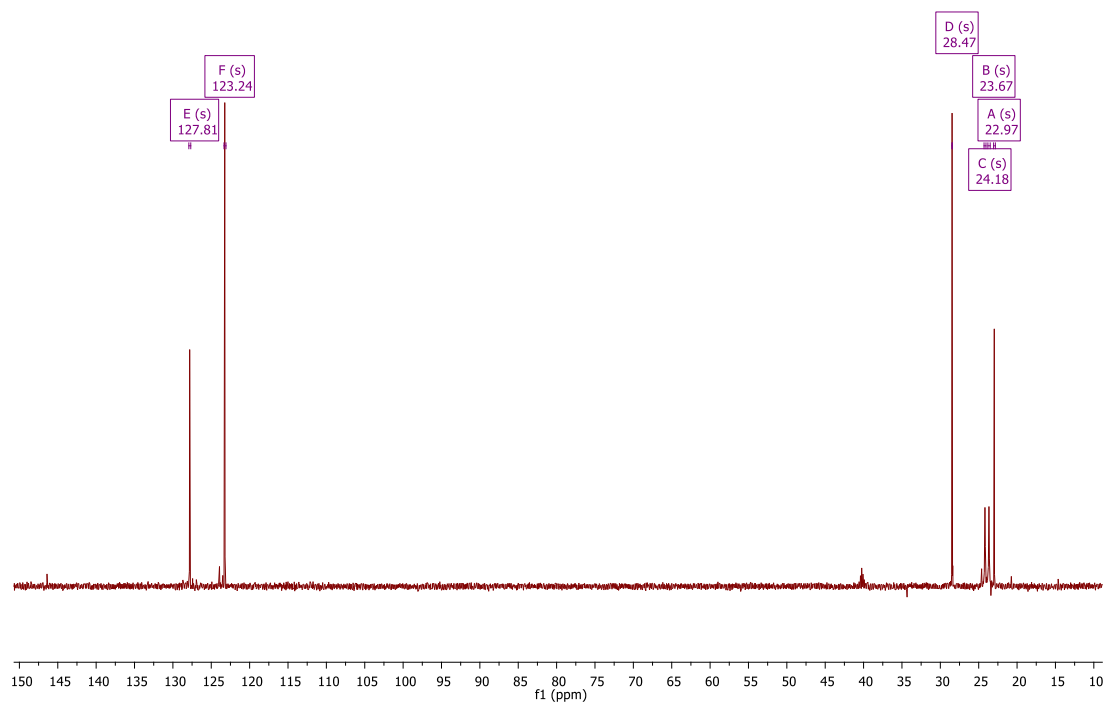


Figure S4. DEPT-135-NMR spectrum of N-(2,6-diisopropylphenyl)acetamide **4** in DMSO.

N-(2,6-diisopropylphenyl)acetamide-DMSO-d₆- ^{13}C

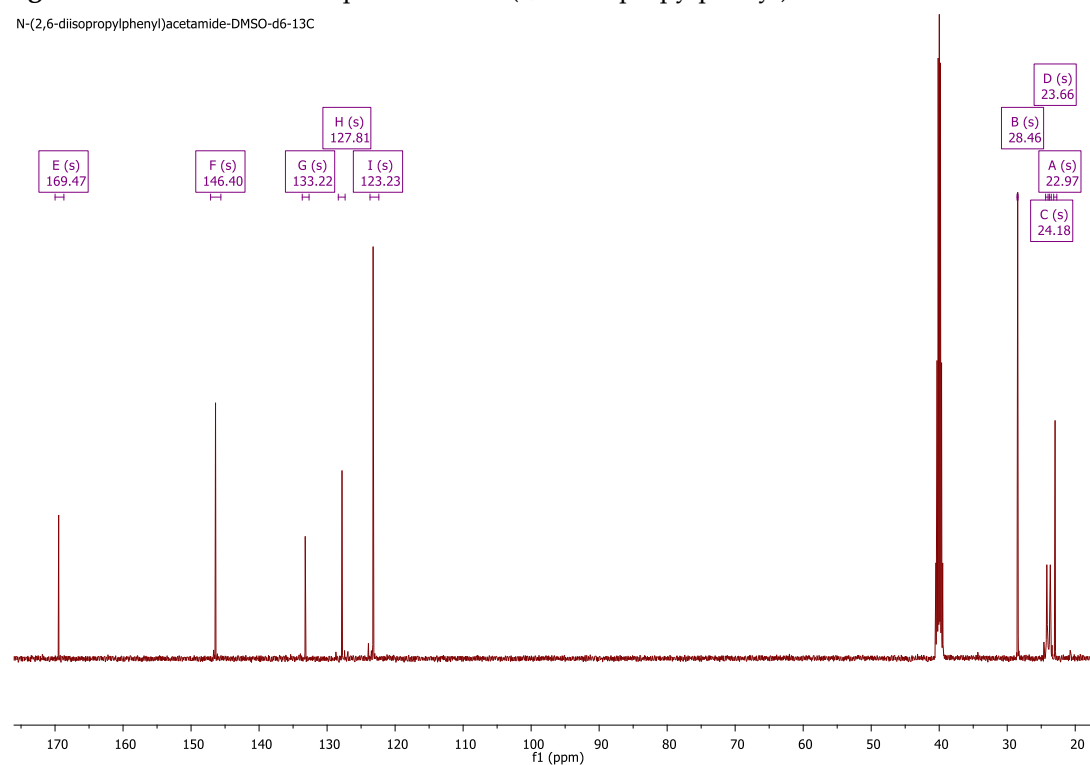


Figure S5. ^{13}C -NMR spectrum of N-(2,6-diisopropylphenyl)acetamide **4** in DMSO.

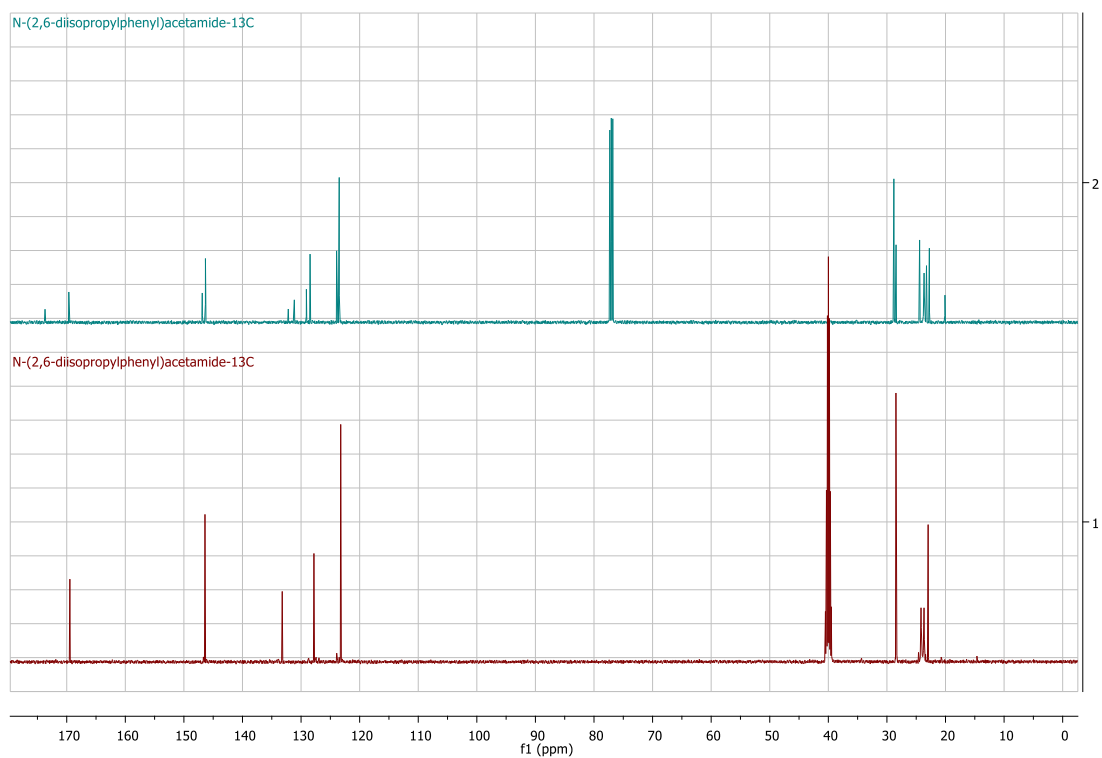


Figure S6. Comparison between ^{13}C -NMR spectra of N-(2,6-diisopropylphenyl)acetamide **4** in deuterated CDCl_3 (blue coloured) and DMSO (red coloured).

NMR ^1H -spectra of compound **2**

N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide-chloroform

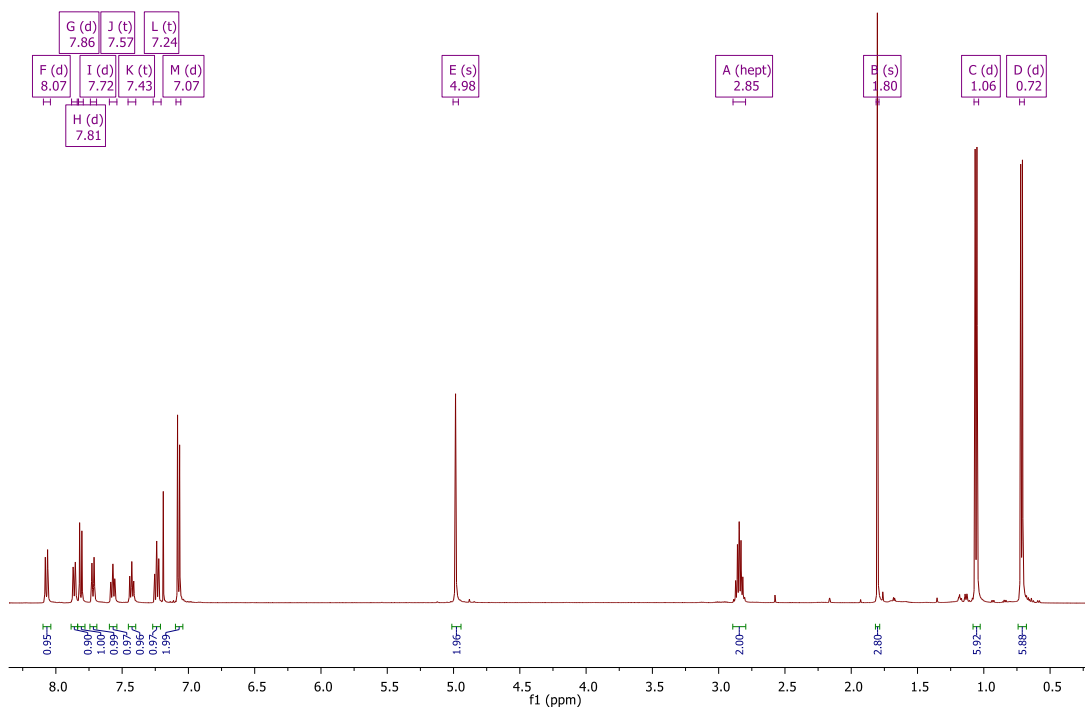


Figure S7. ^1H -NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl_3 .

N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide-chloroform

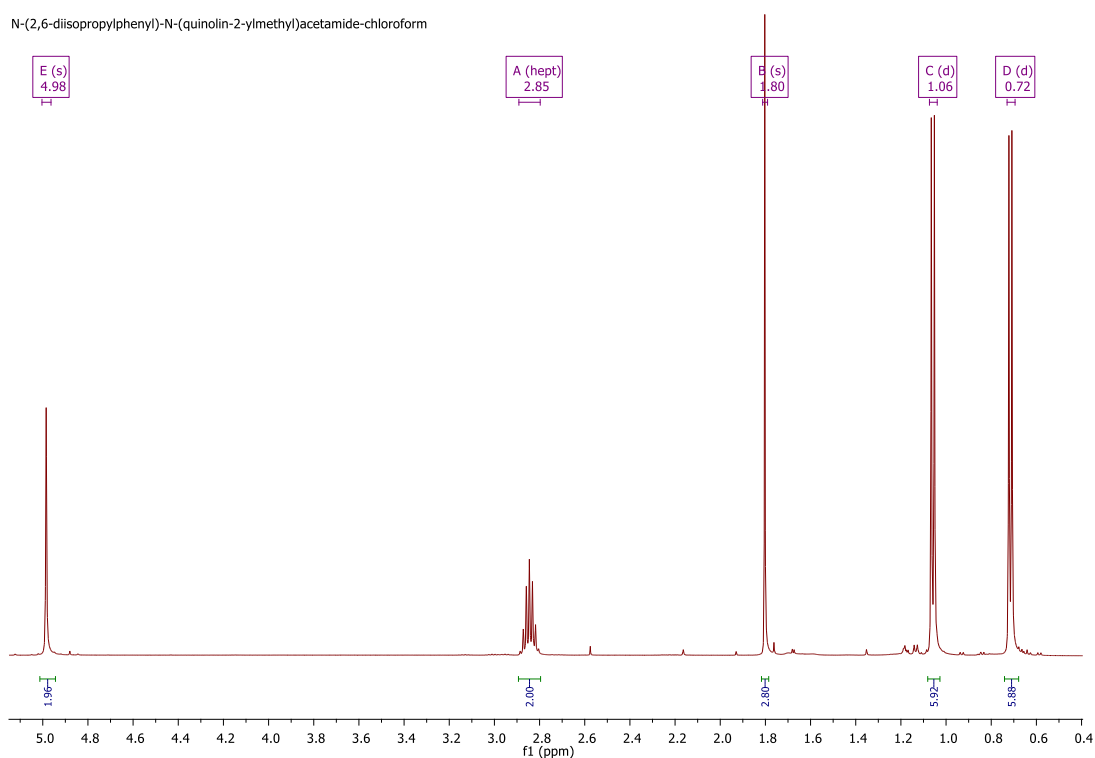


Figure S8. ^1H -NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl_3 at the 0.6-5.0 ppm region.

N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide-chloroform

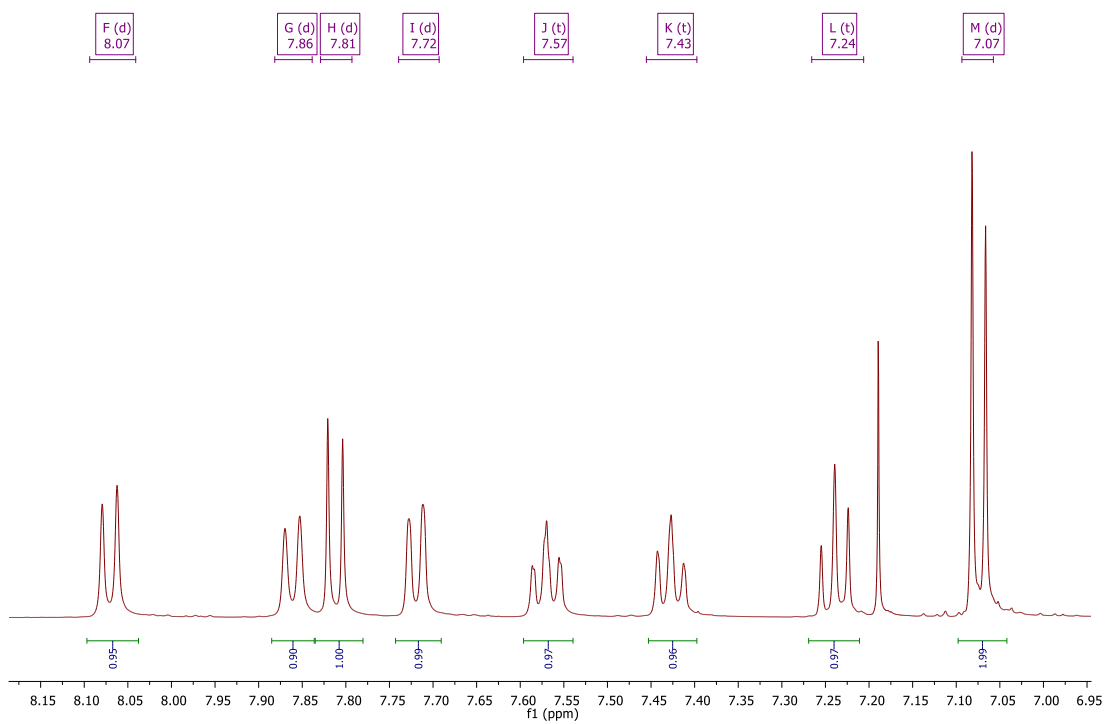


Figure S9. ¹H-NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl₃ at the 7.00-8.10 ppm region.

NMR ^{13}C -spectra of compound **2**

N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide-DEPT-135

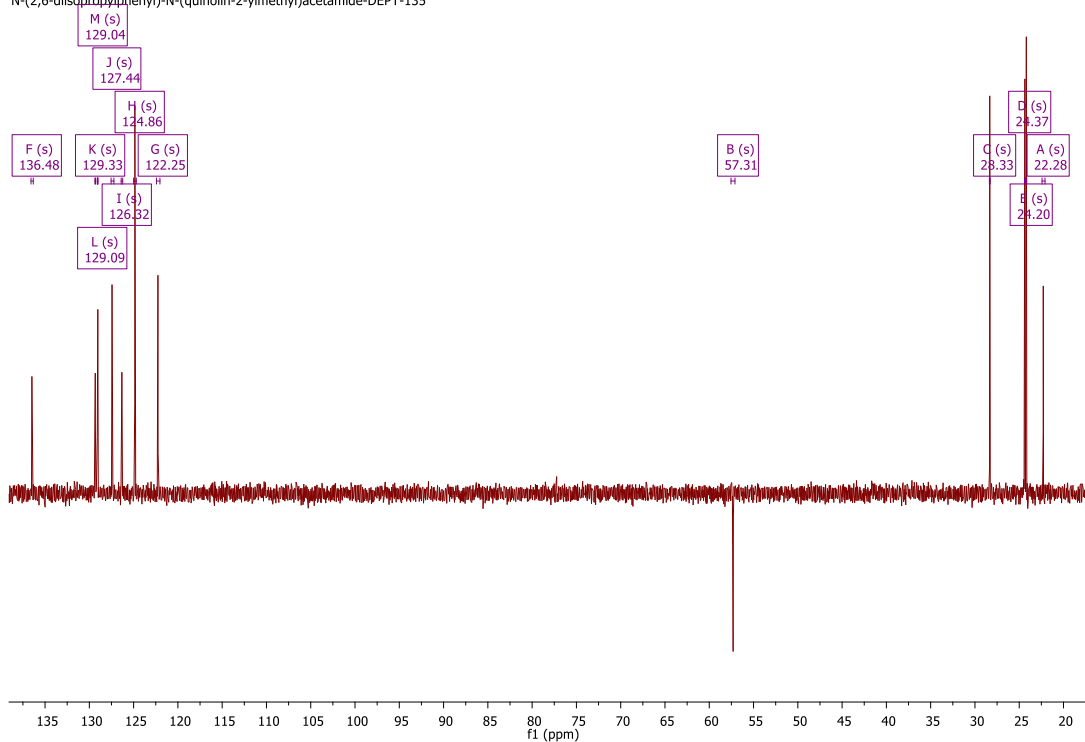


Figure S10. DEPT-135-NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl_3 .

N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide-DEPT-135

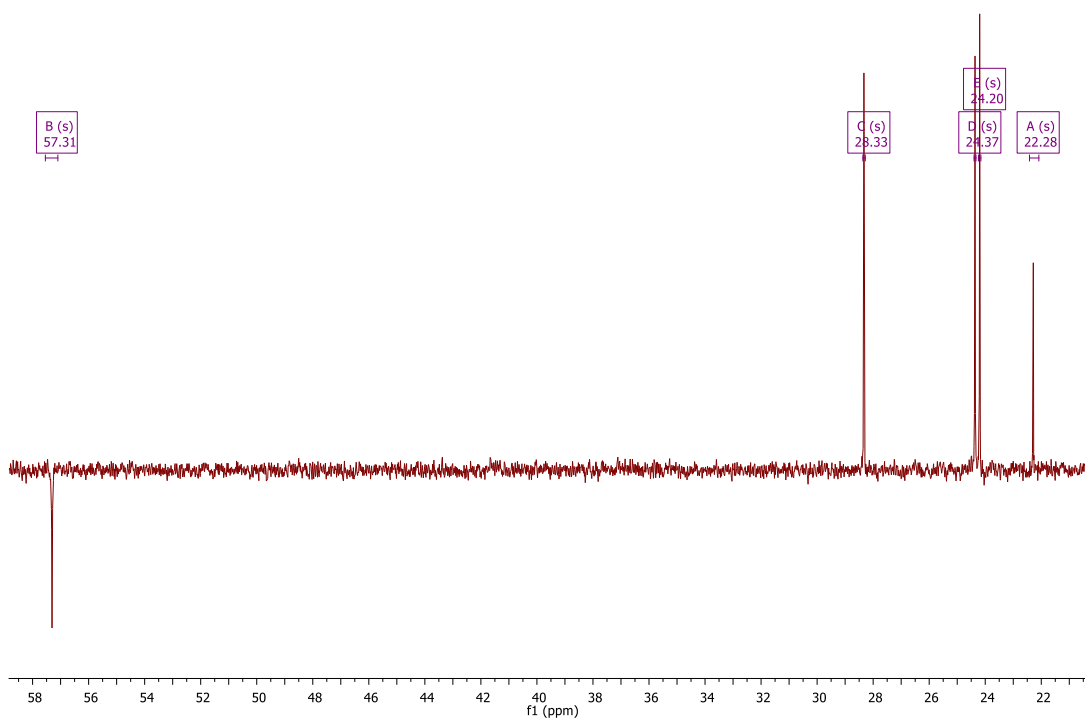


Figure S11. DEPT-135-NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl_3 at the 22.00-58.00 ppm region.

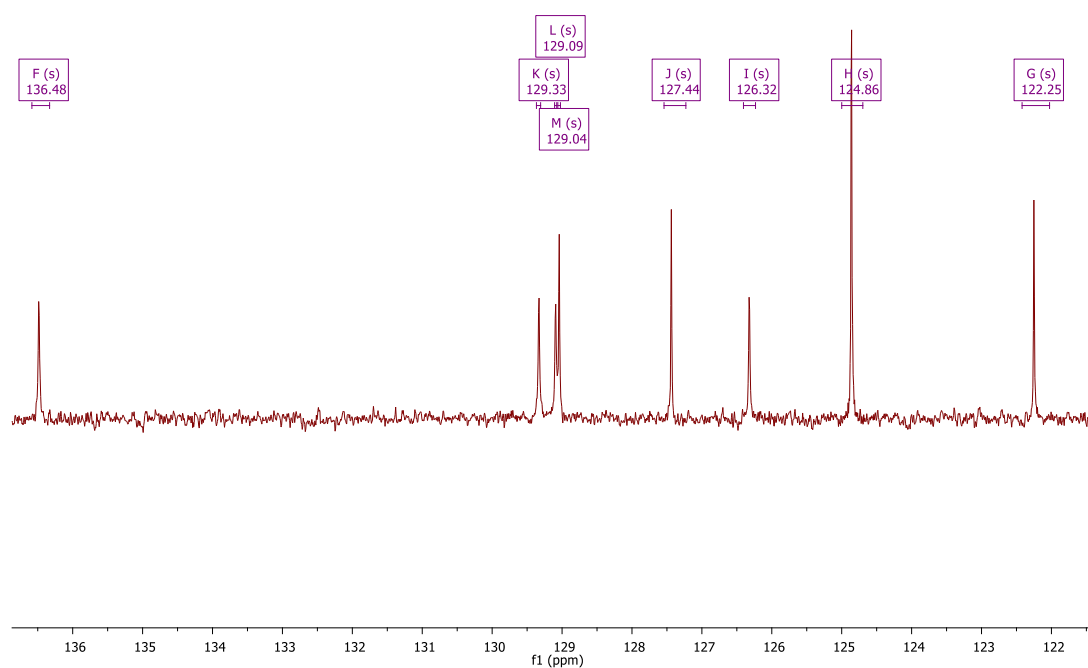


Figure S12. DEPT-135-NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl₃ at the 122.00-137.00 ppm region.

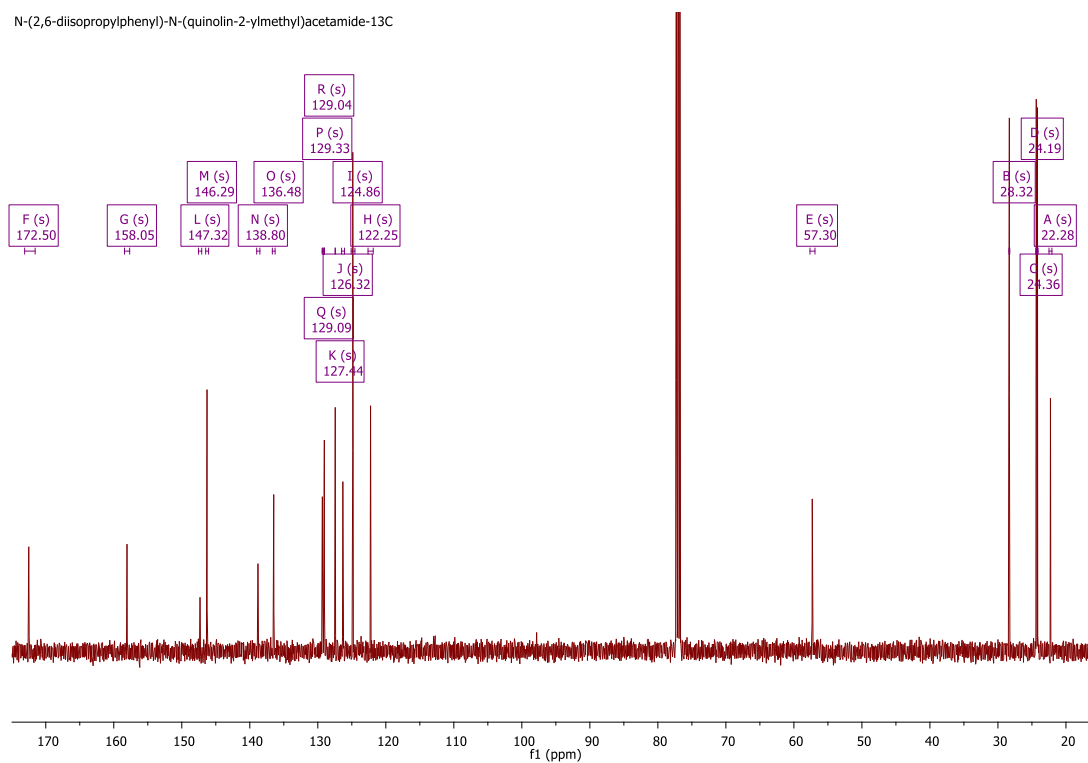


Figure S13. ¹³C-NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl₃.

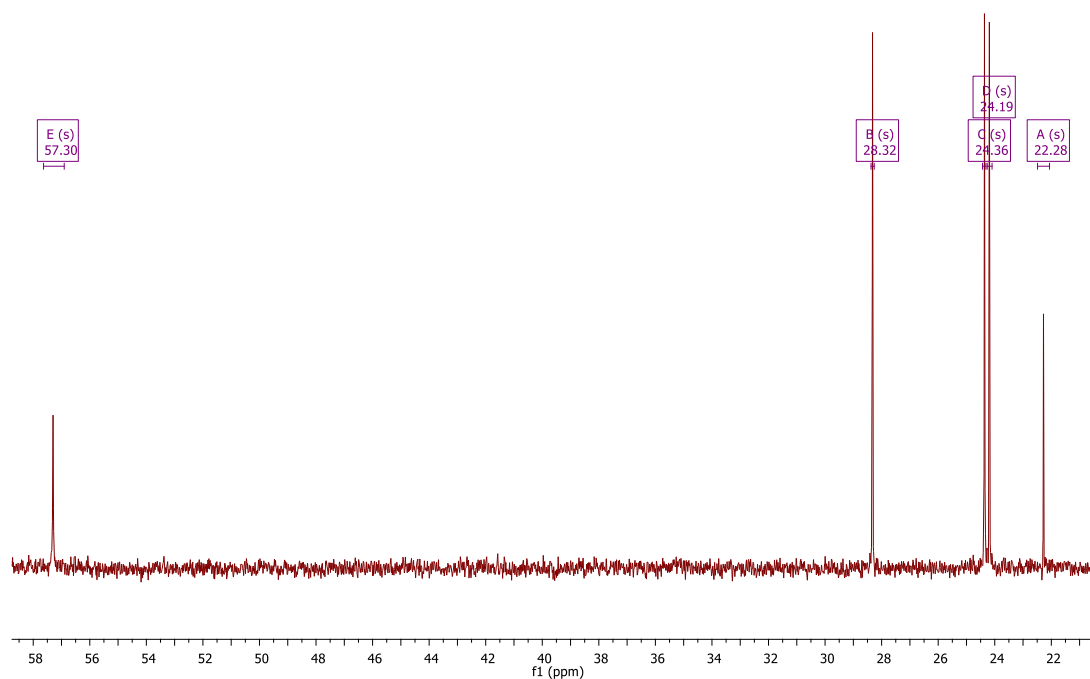


Figure S14. ^{13}C -NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl_3 at the 22.00-58.00 ppm region.

N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide-13C

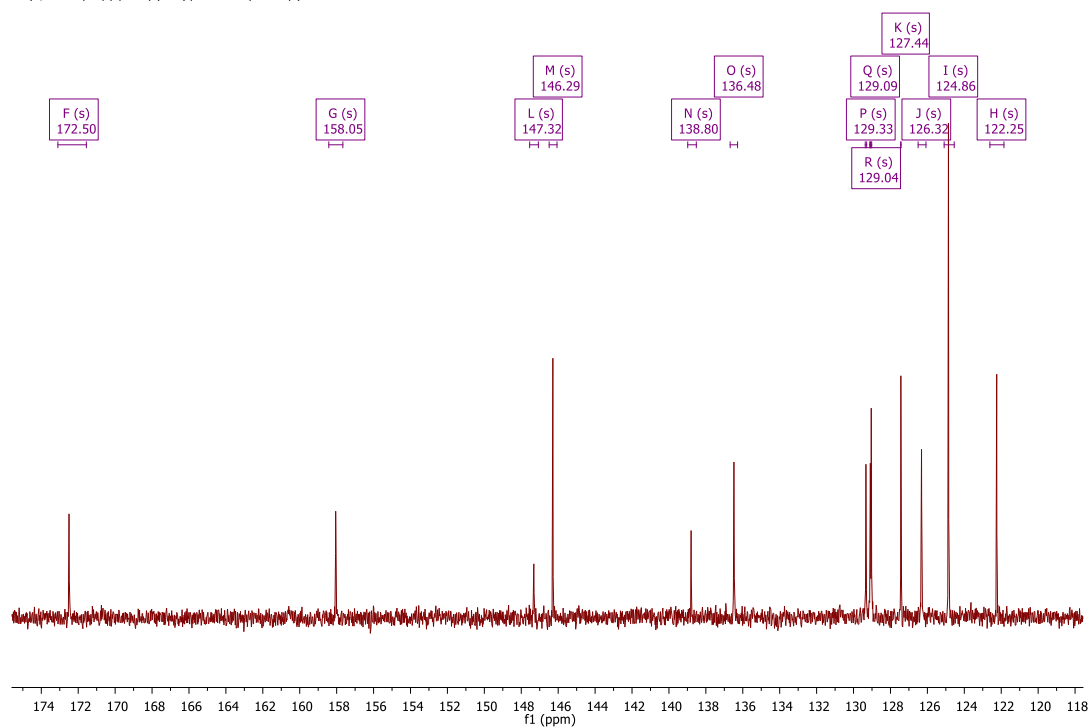


Figure S15. ^{13}C -NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl_3 at the 122.00-174.00 ppm region.

NMR 2D spectra – COSY, HSQC, HMBS of compound **2**

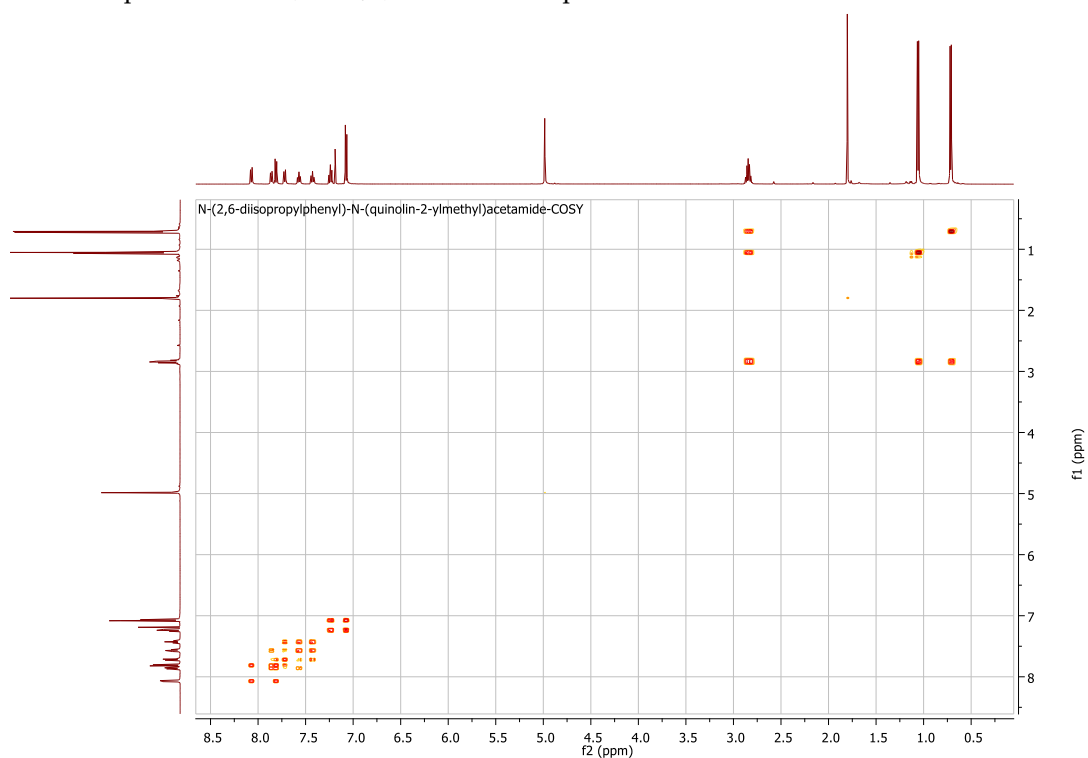


Figure S16. COSY NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl₃.

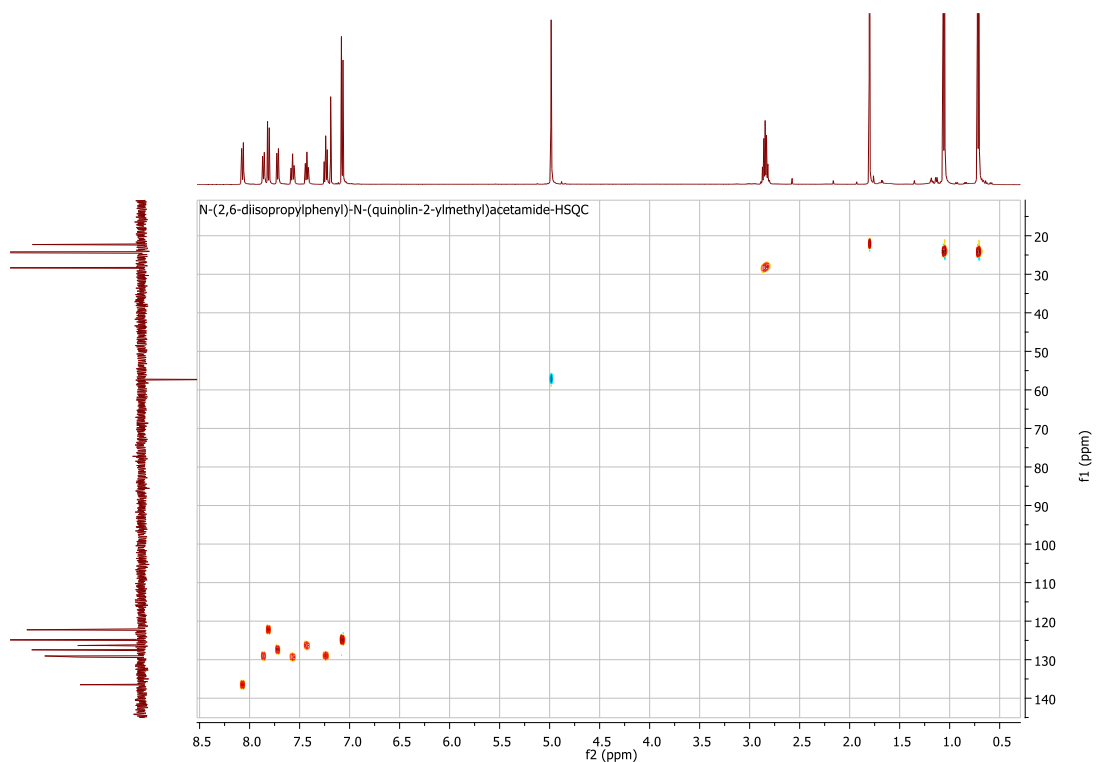


Figure S17. HSQC NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl₃.

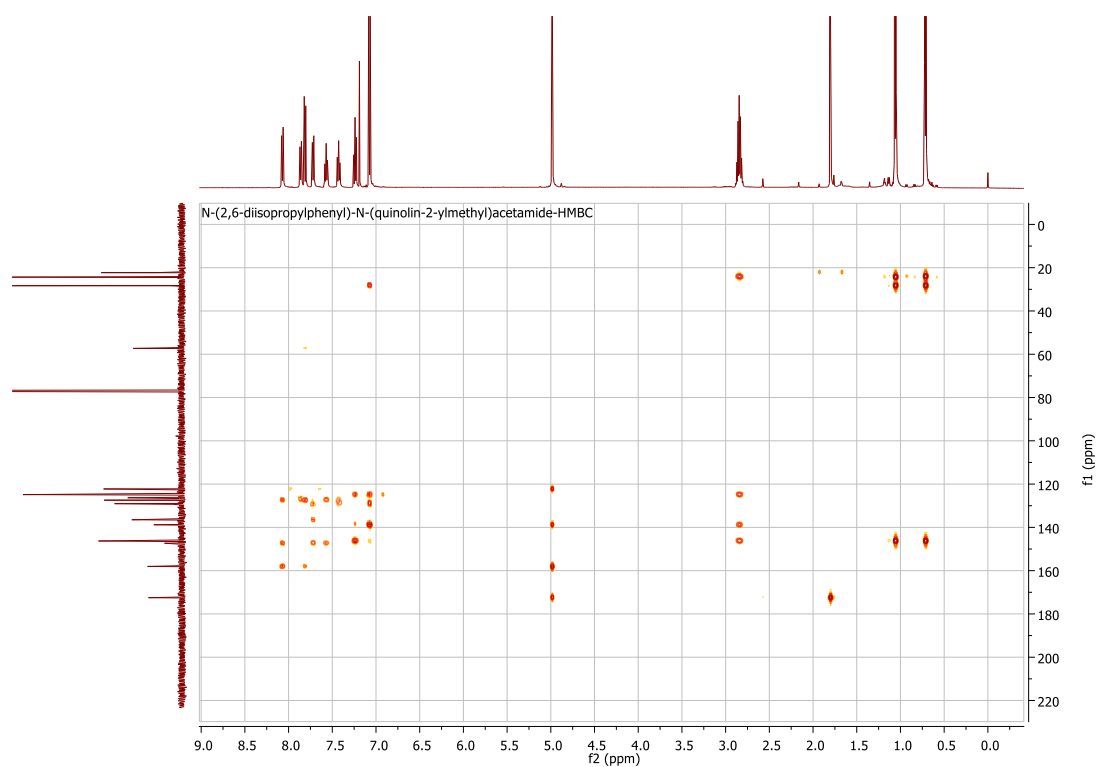


Figure S18. HMBC NMR spectrum of N-(2,6-diisopropylphenyl)-N-(quinolin-2-ylmethyl)acetamide **2** in CDCl₃.

NMR ^1H and ^{13}C -spectra of compound **1** in DMSO

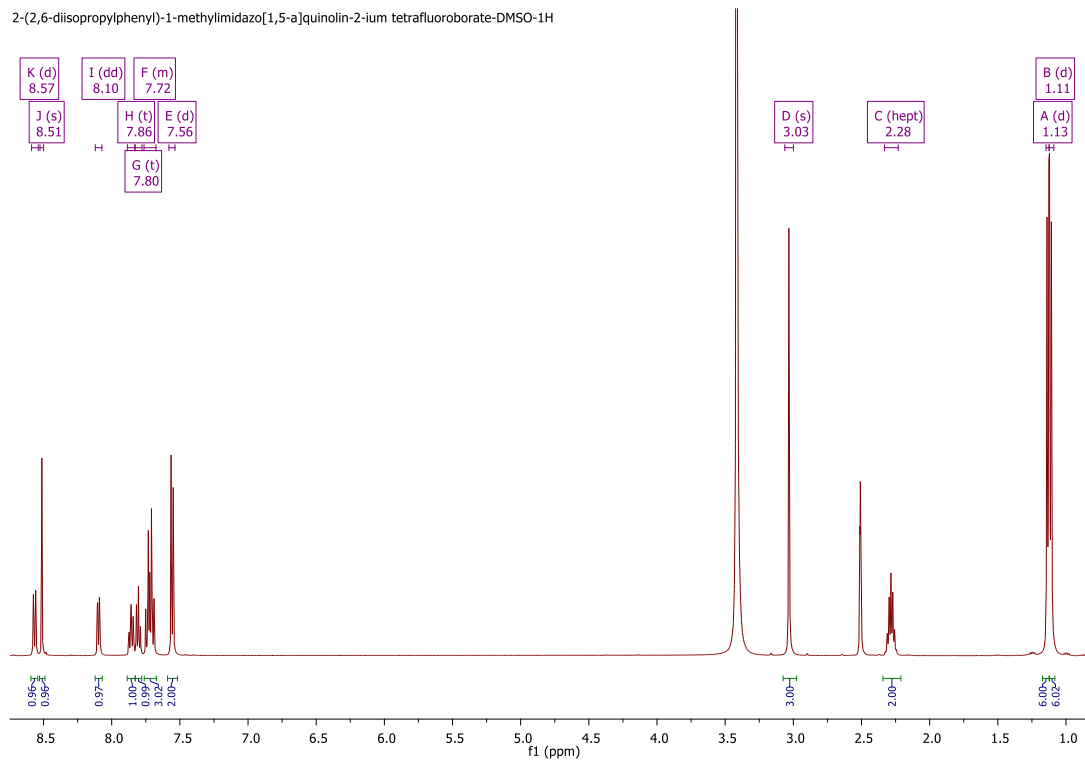


Figure S19. ^1H -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO.

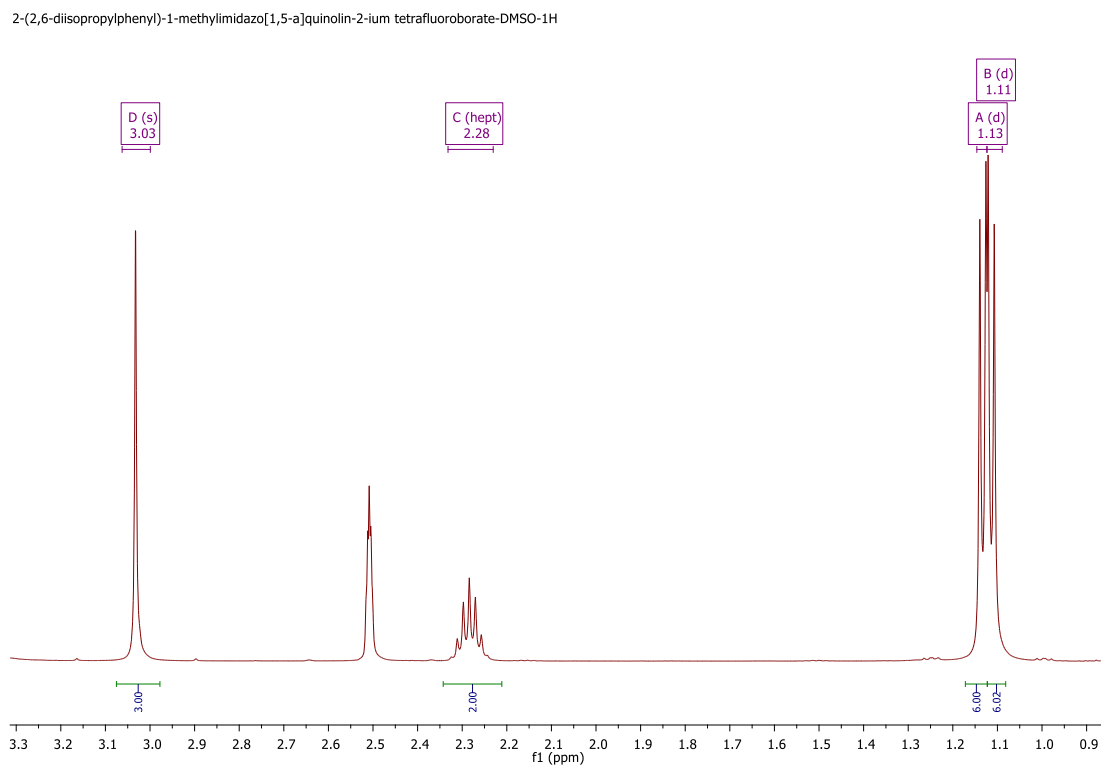


Figure S20. ^1H -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO at the 1.0-3.1 ppm region.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-DMSO-1H

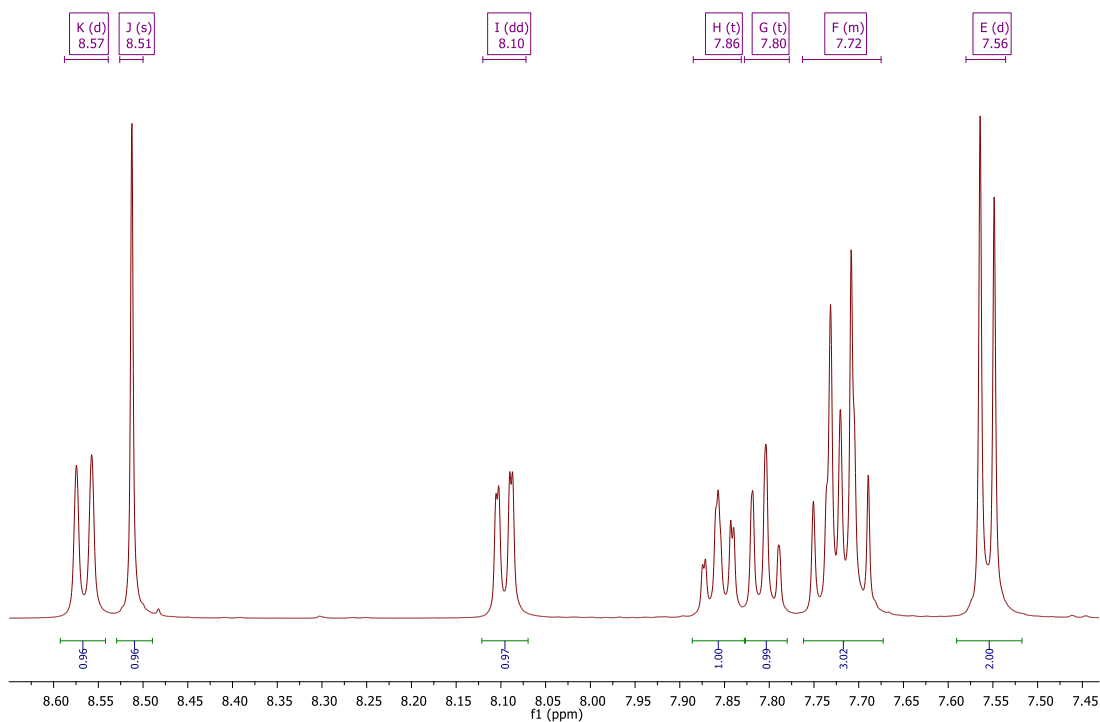


Figure S21. ^1H -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO at the 7.50-8.60 ppm region.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-DMSO-DEPT-135

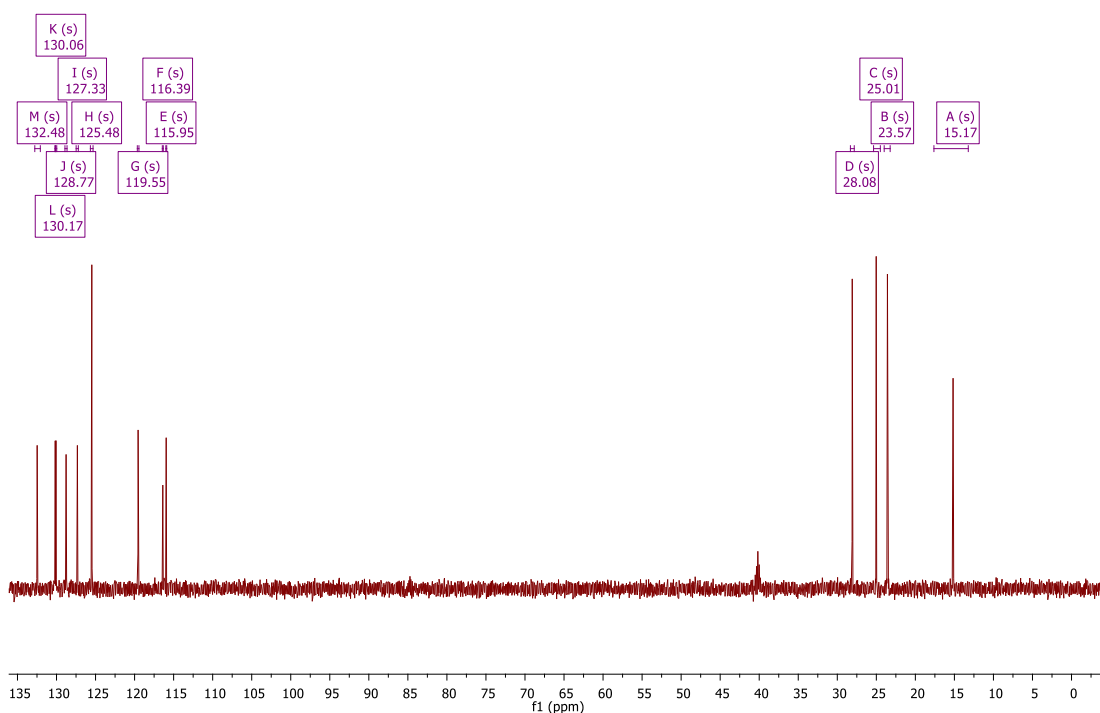


Figure S22. DEPT-135-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO.

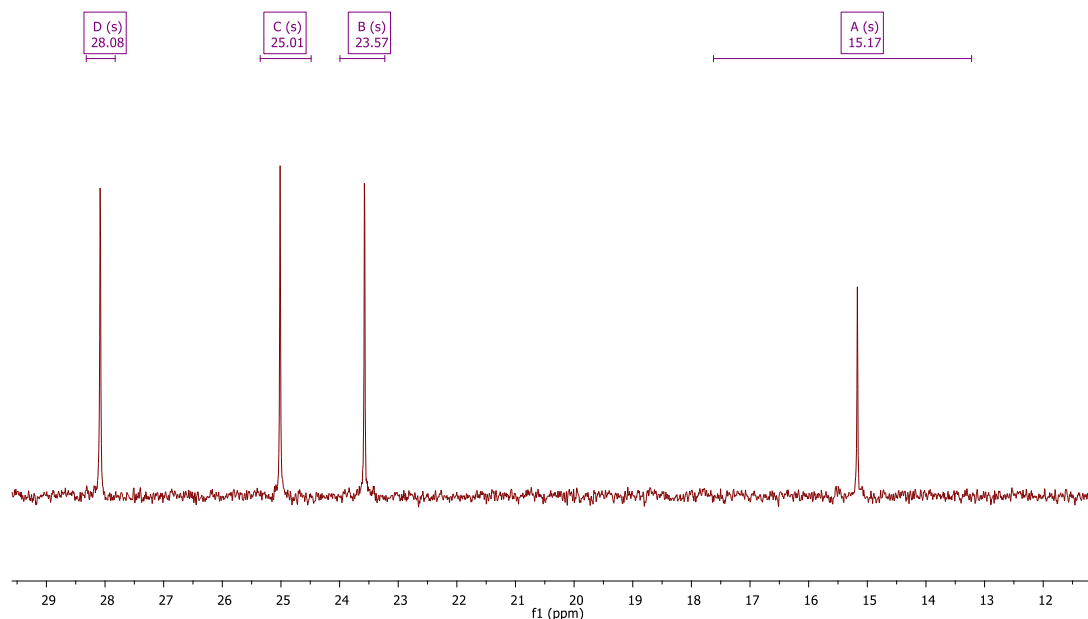


Figure S23. DEPT-135-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO at the 12.00-29.00 ppm region.

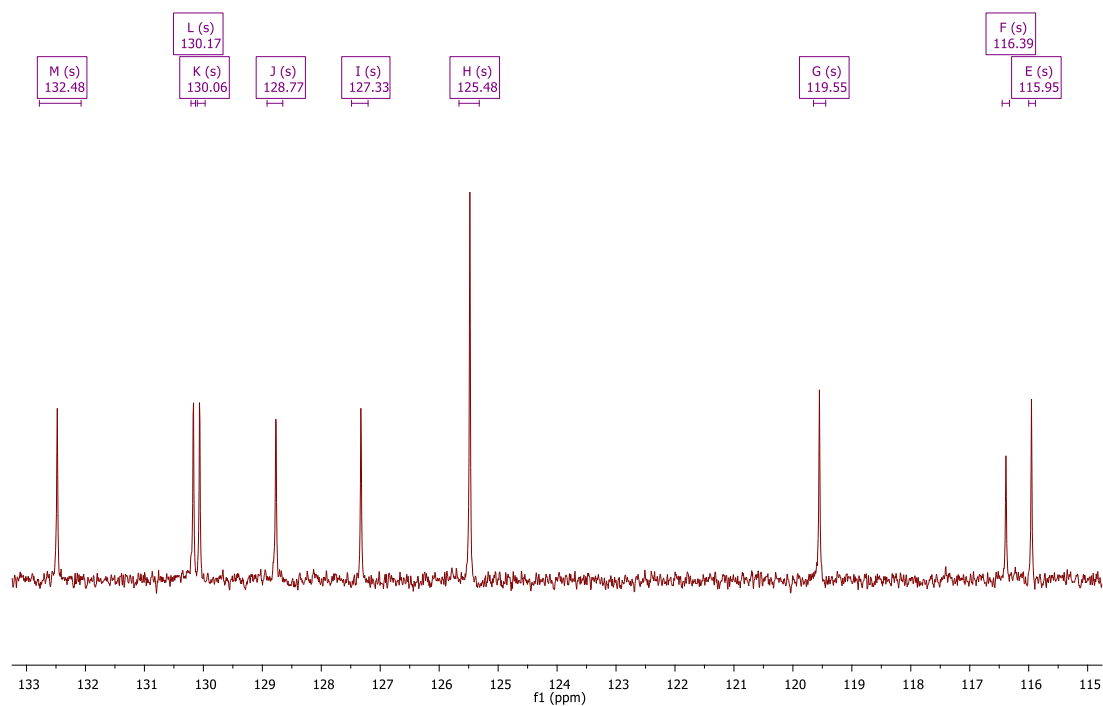


Figure S24. DEPT-135-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO at the 115.00-133.00 ppm region.

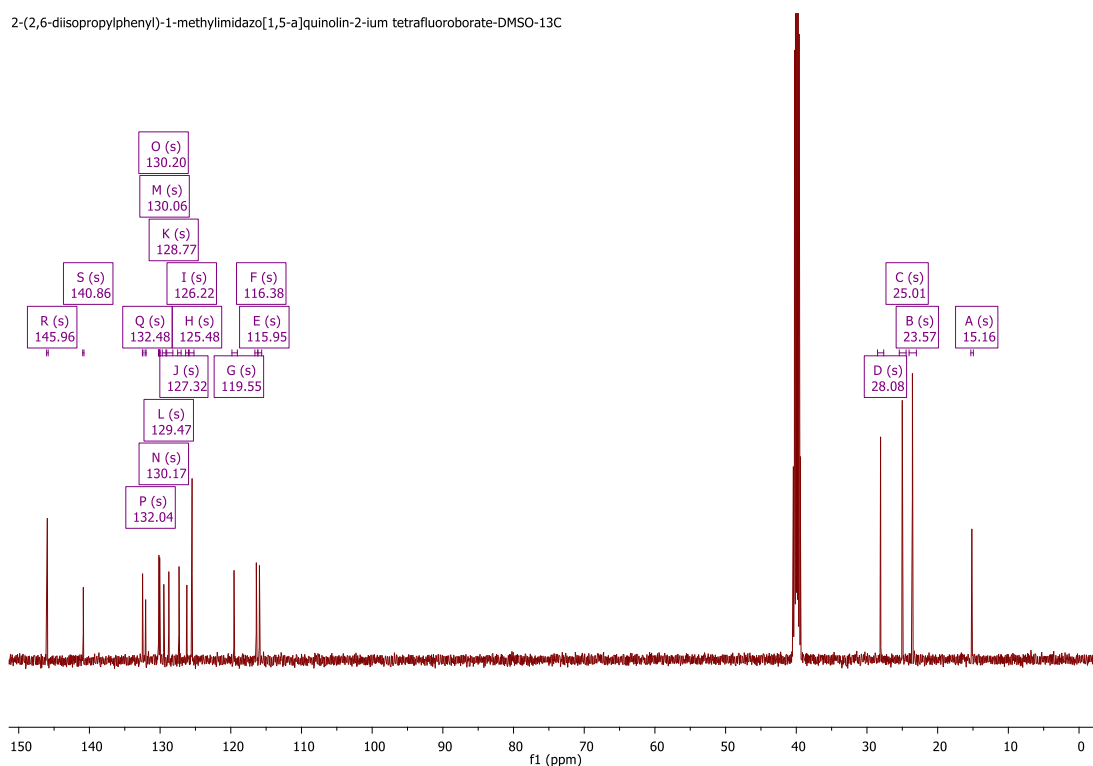


Figure S25. ^{13}C -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO.

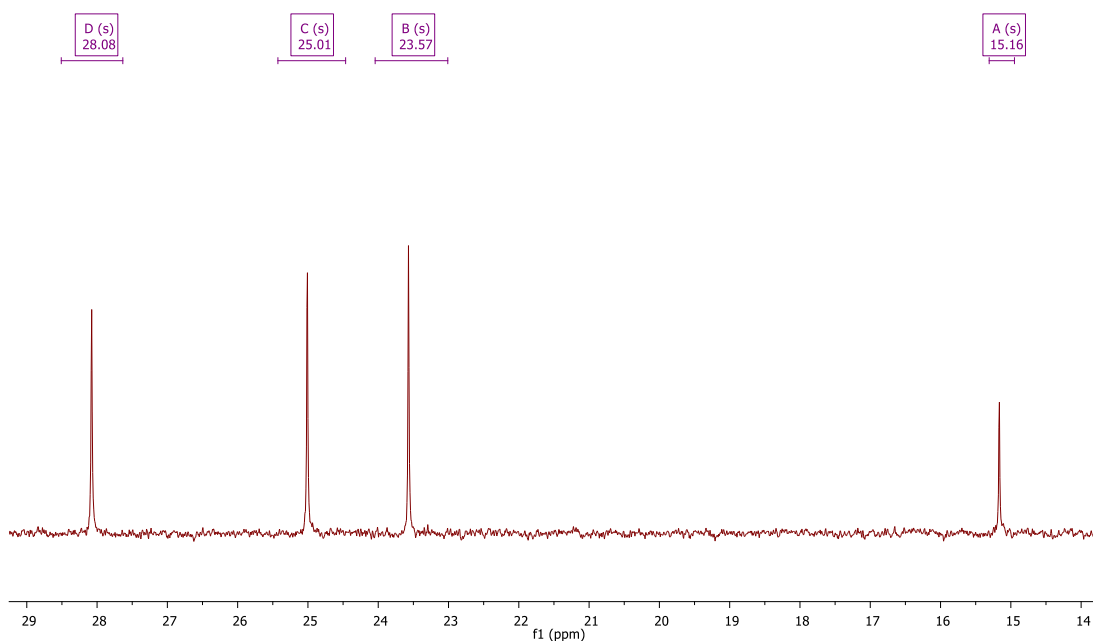


Figure S26. ^{13}C -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO at the 15.00-29.00 ppm region.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-DMSO-13C

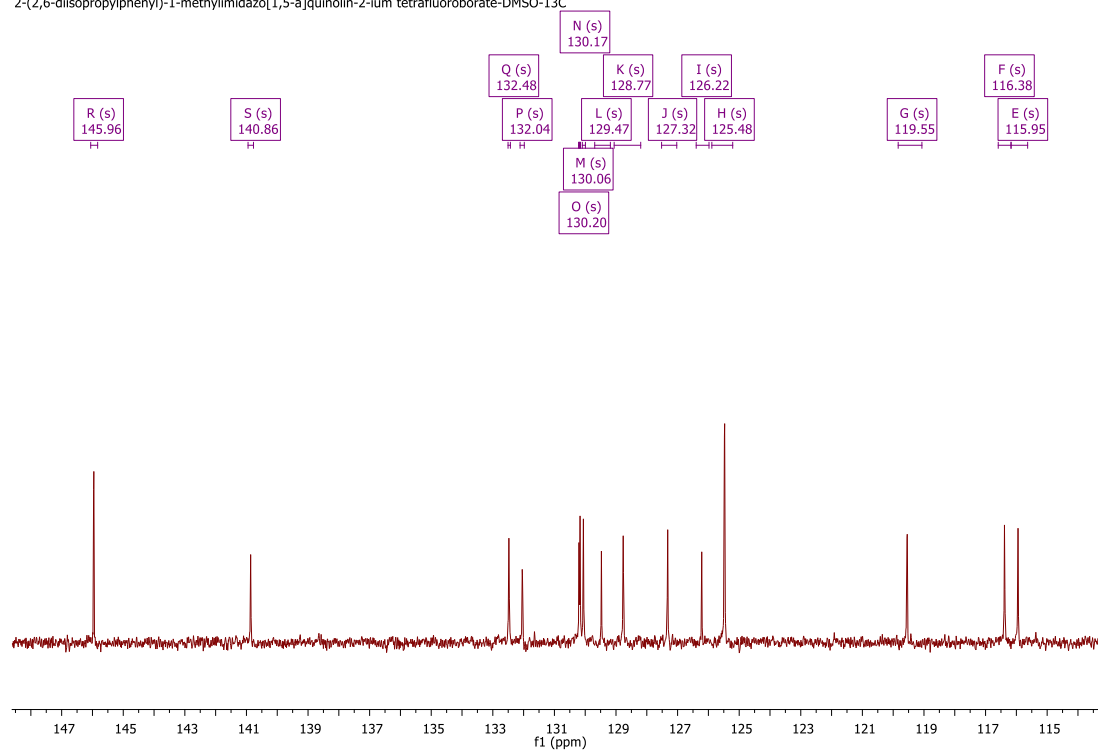


Figure S27. ^{13}C -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO at the 115.00-147.00 ppm region.

NMR 2D spectra – COSY, HSQC, HMBS of compound **1** in DMSO

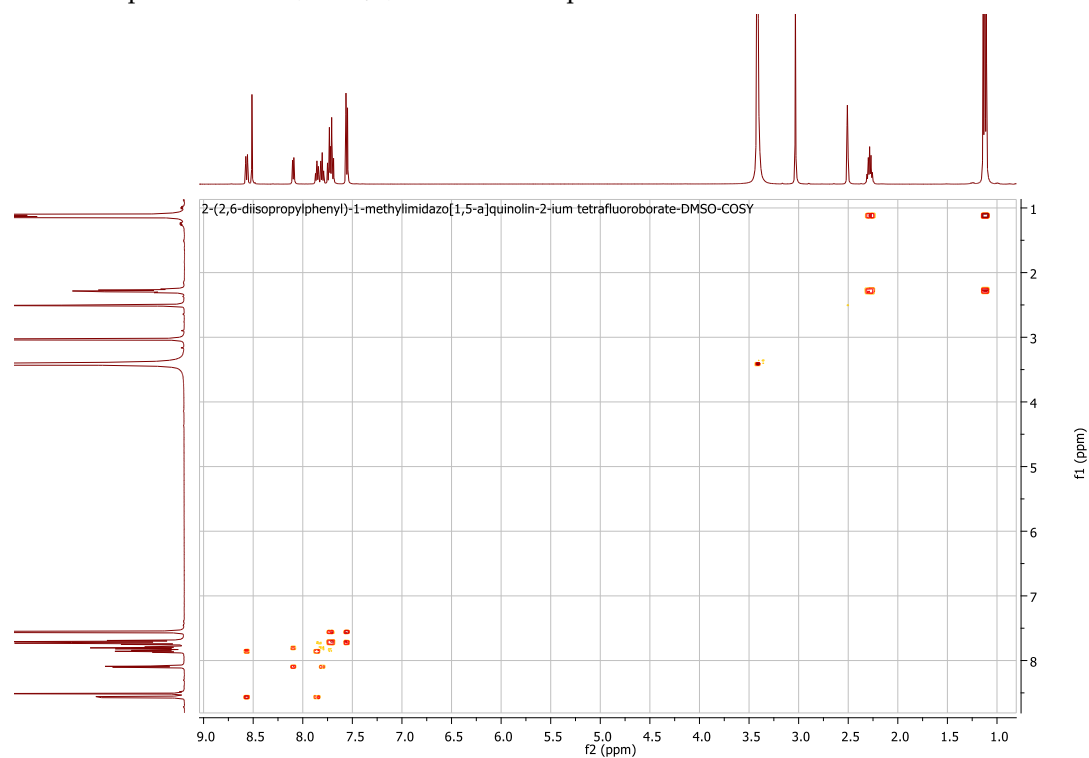


Figure S28. COSY-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO.

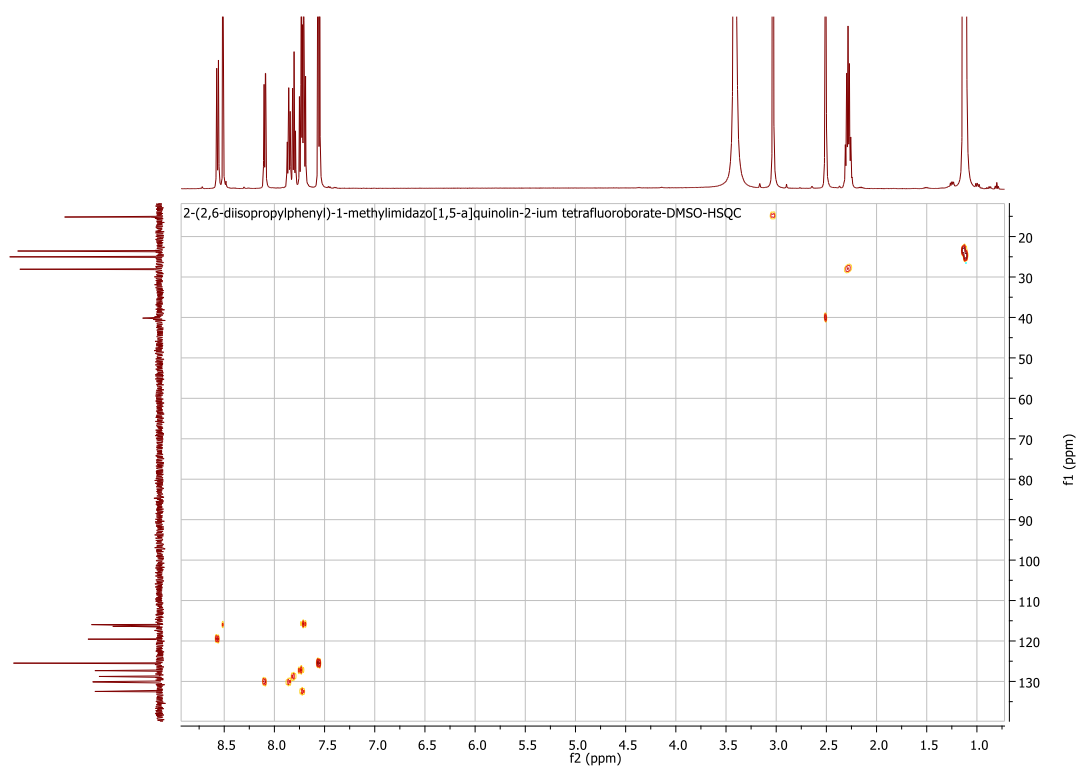


Figure S29. HSQC-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO.

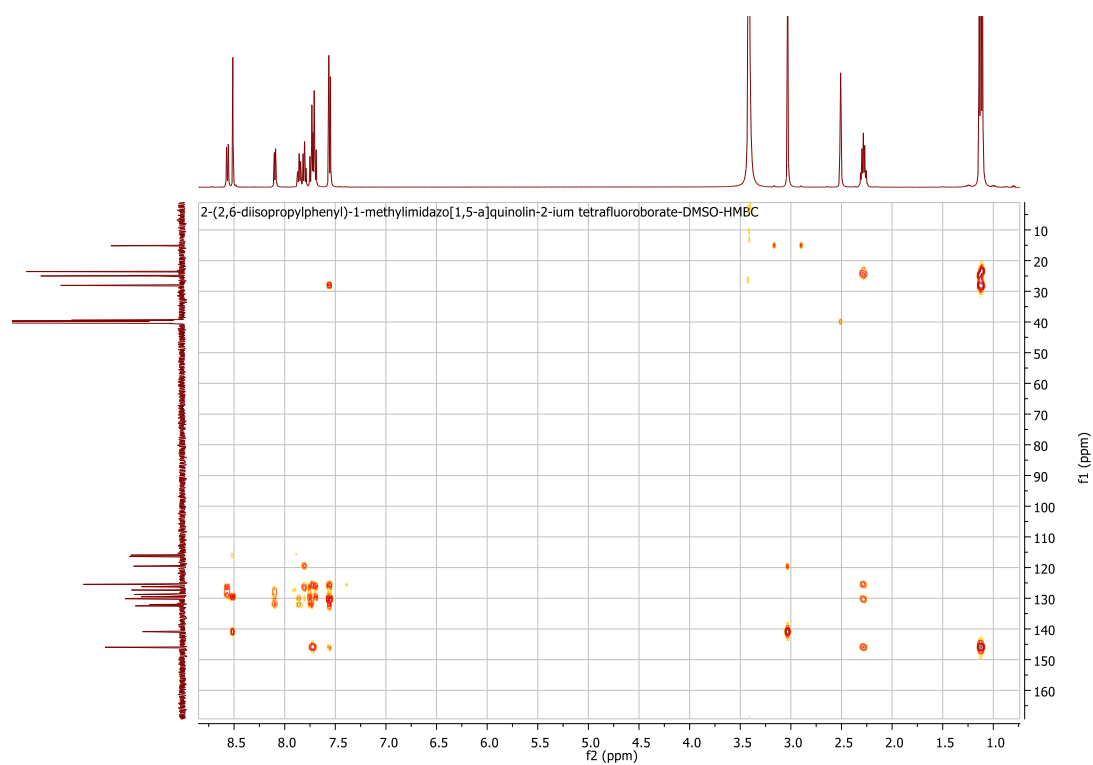


Figure S30. HMBC-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in DMSO.

NMR ^1H and ^{13}C -spectra of compound **1** in methanol

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-MeOH-1H

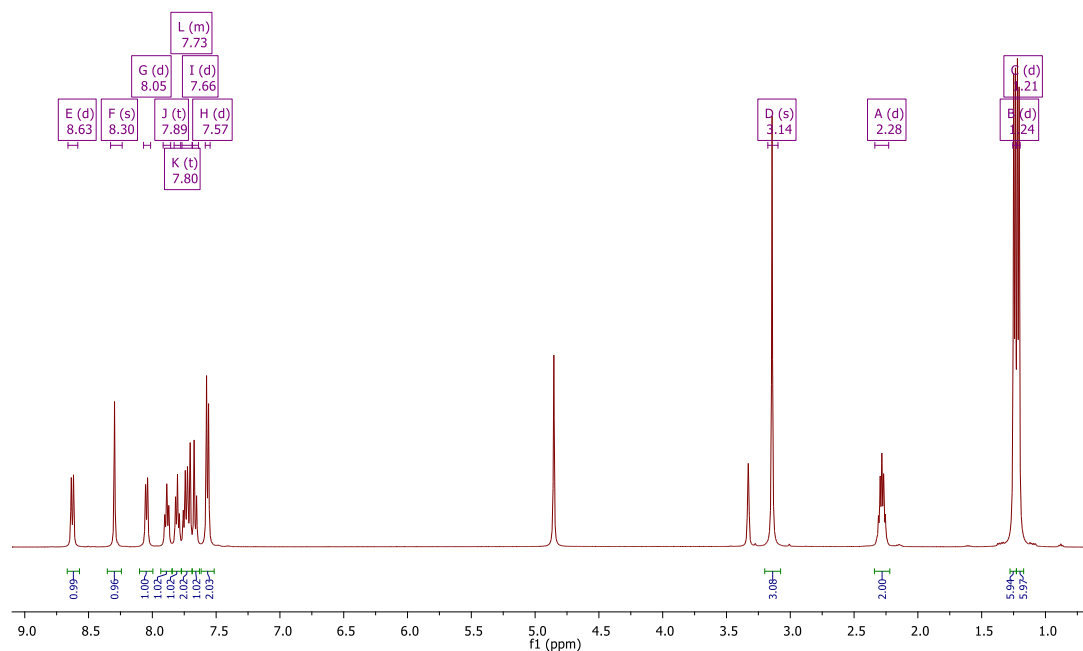


Figure S31. ^1H -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-MeOH-1H

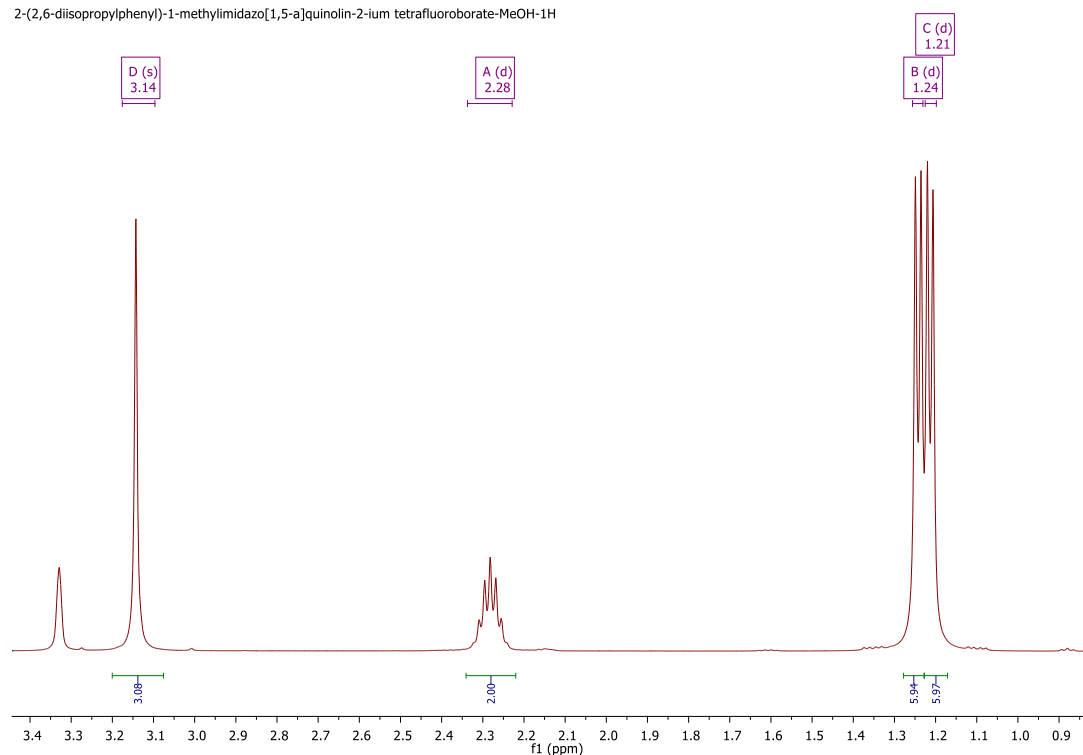


Figure S32. ^1H -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol at the 1.00-3.40 ppm region.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-MeOH-1H

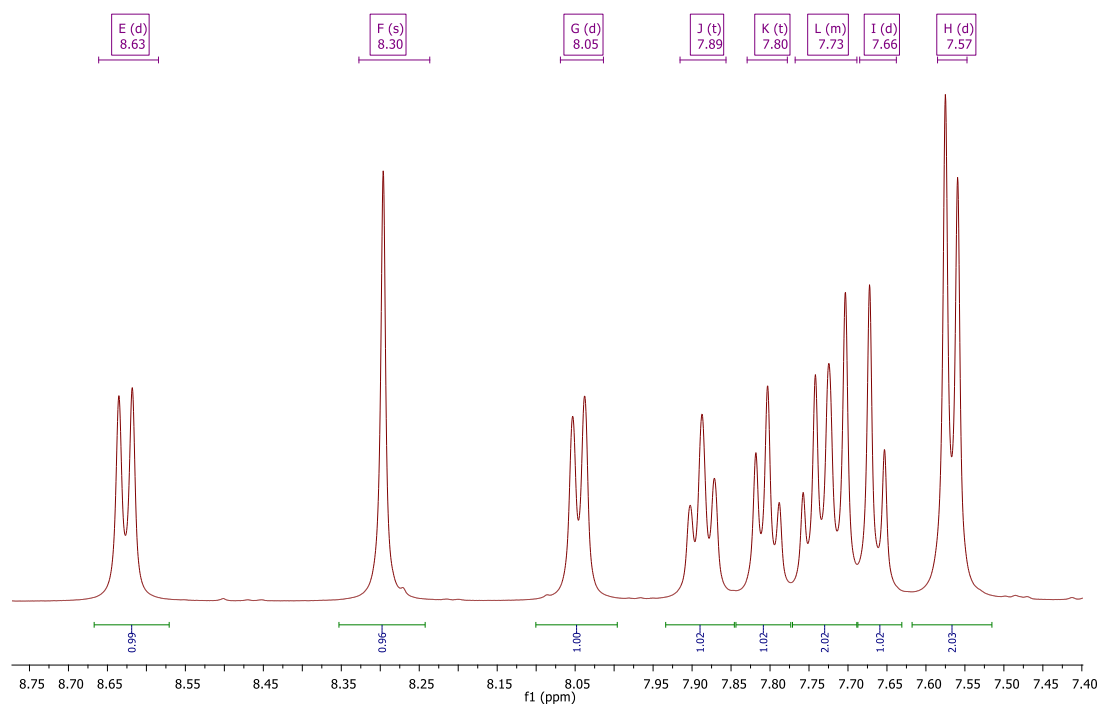


Figure S33. ^1H -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol at the 7.40-8.70 ppm region.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-MeOH-DEPT-135

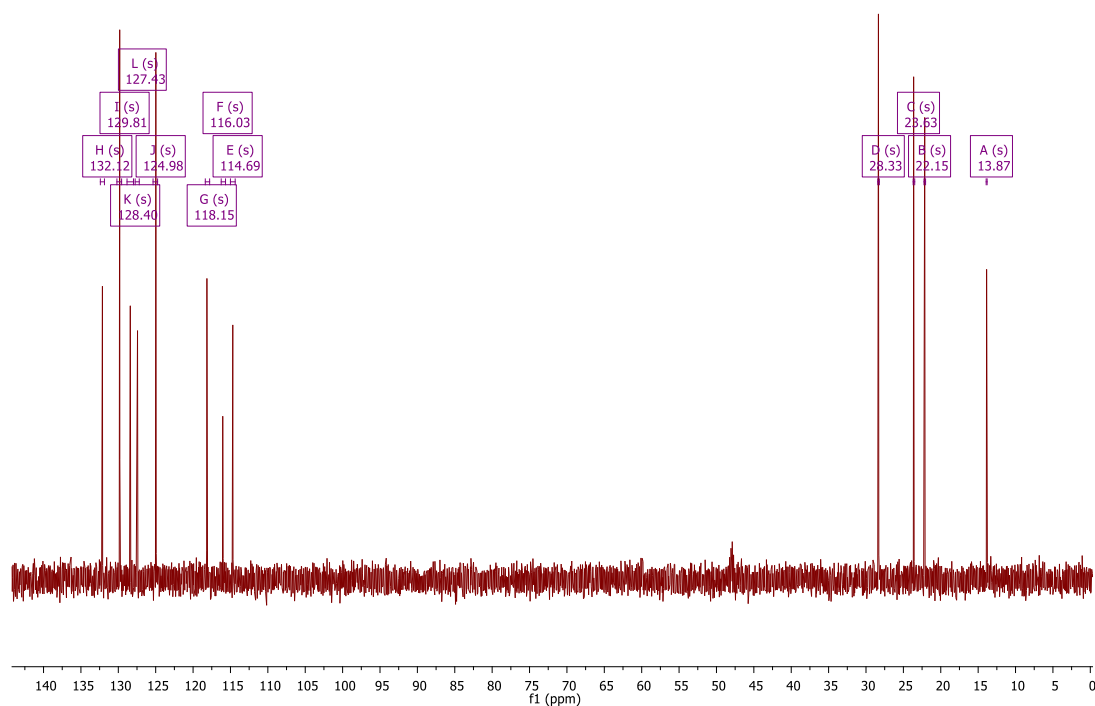


Figure S34. DEPT-135-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol.

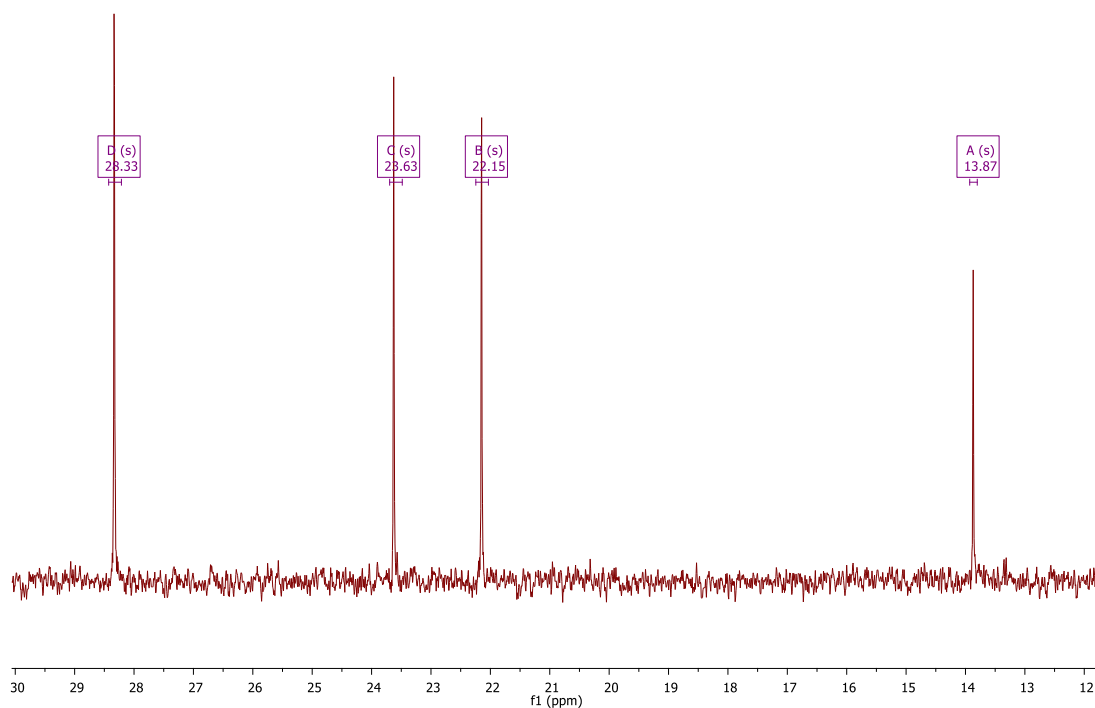


Figure S35. DEPT-135-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol at the 13.00-29.00 ppm region.

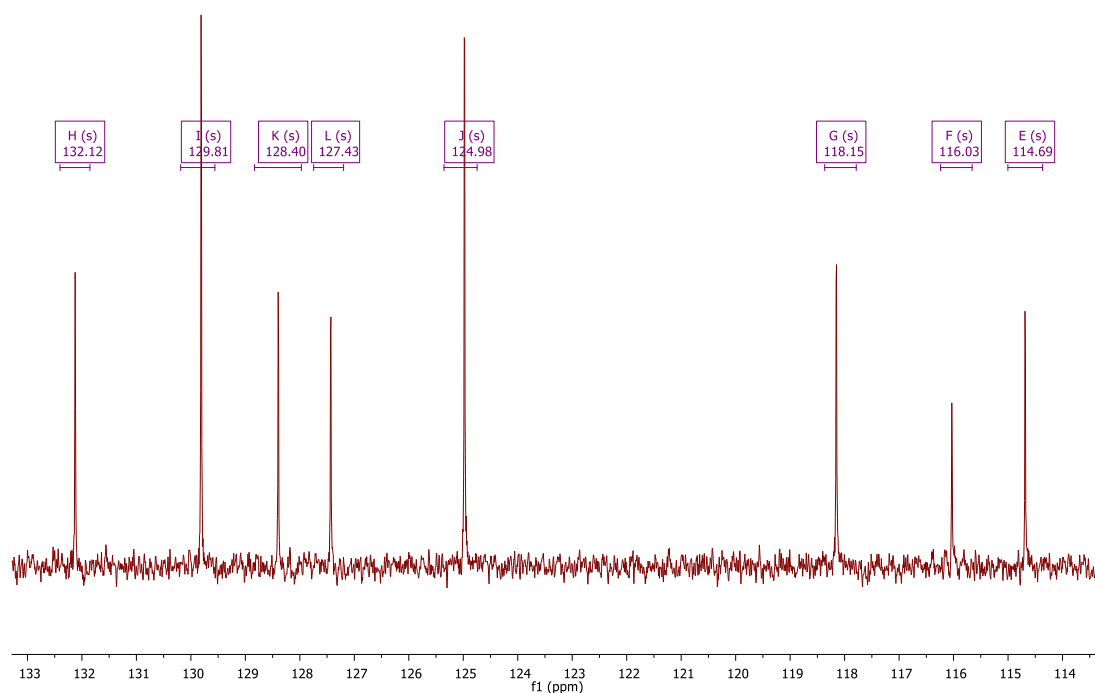


Figure S36. DEPT-135-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol at the 114.00-133.00 ppm region.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-MeOH-13C

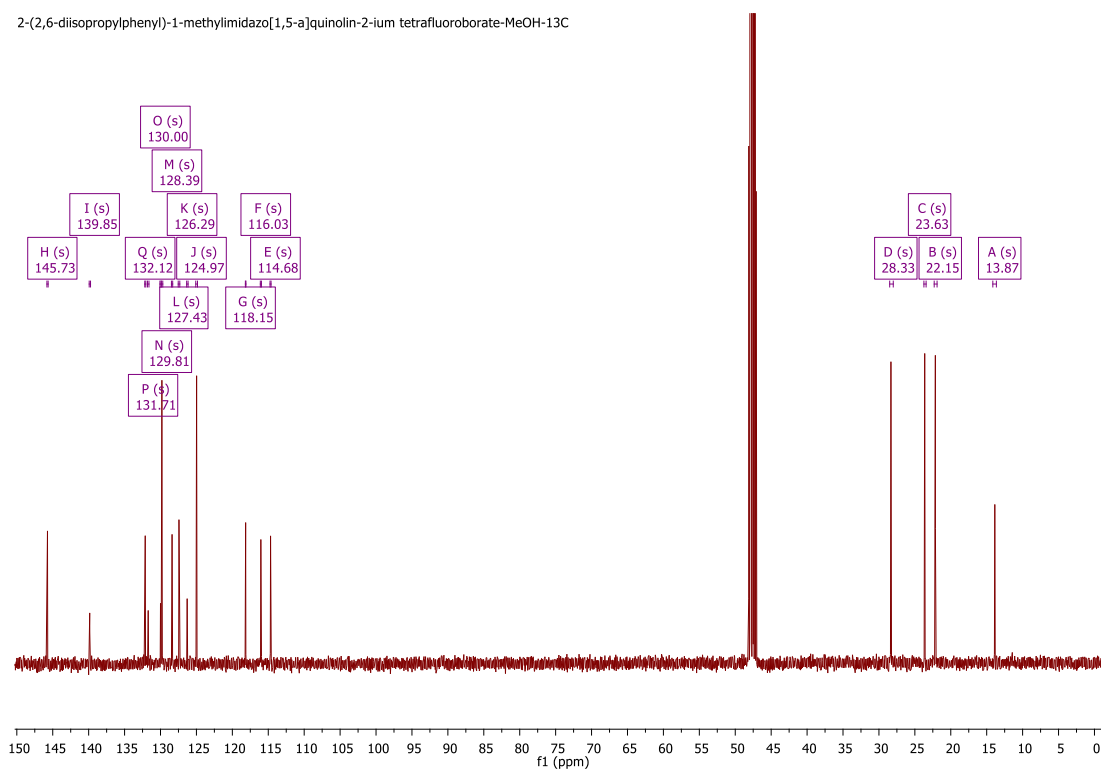


Figure S37. ^{13}C -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol.

2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate-MeOH-13C

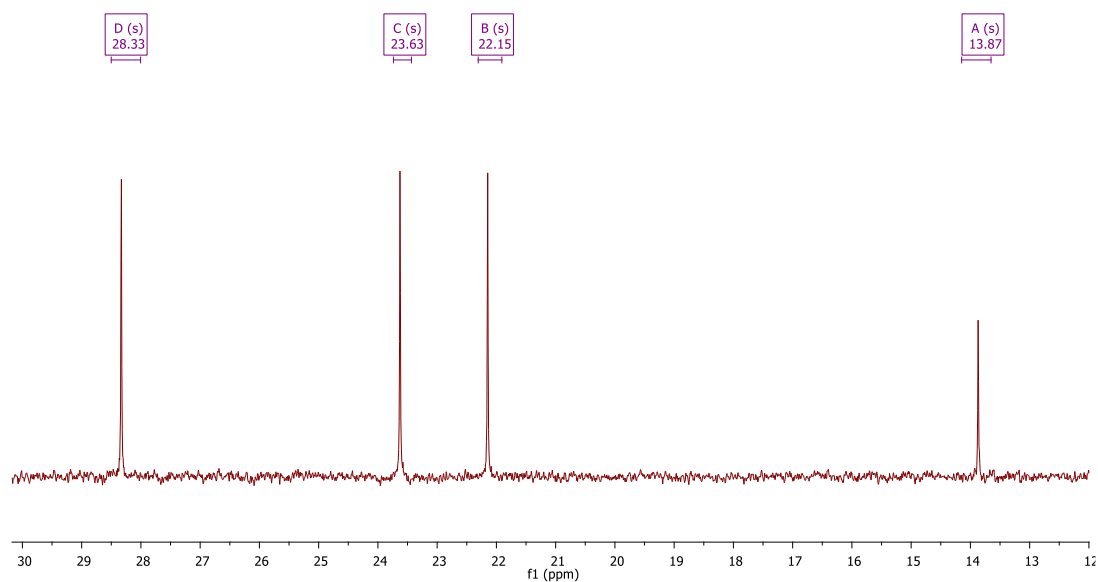


Figure S38. ^{13}C -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol at the 13.00-29.00 ppm region.

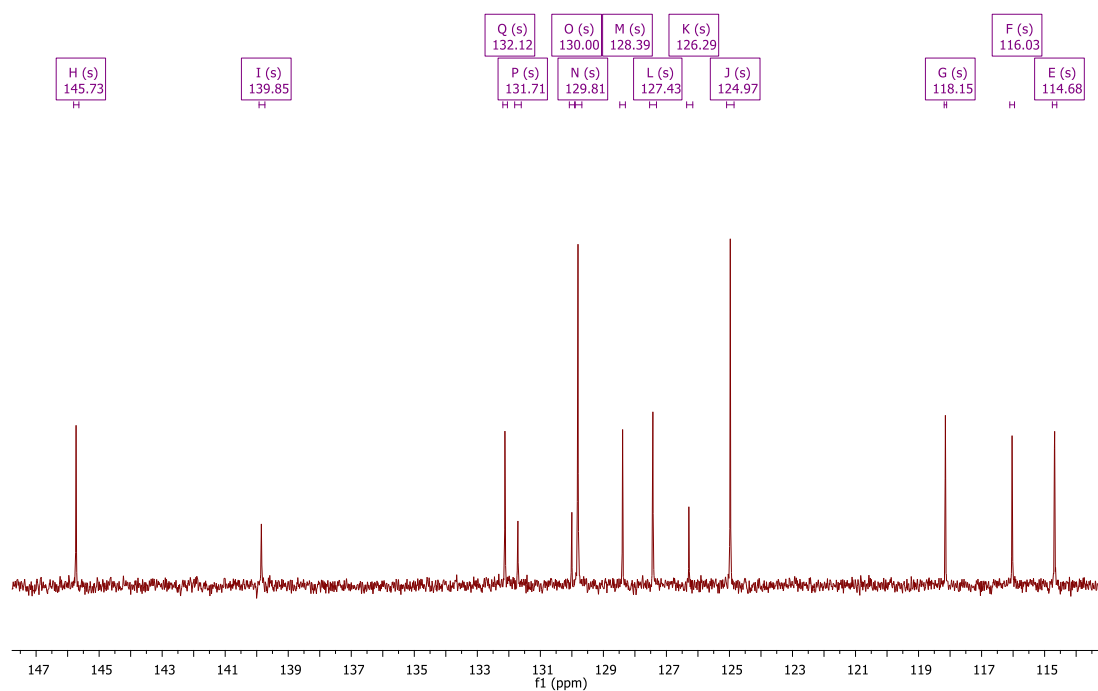


Figure S39. ^{13}C -NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol at the 114.00-147.00 ppm region.

NMR 2D spectra – COSY, HSQC, HMBS of compound **1** in methanol

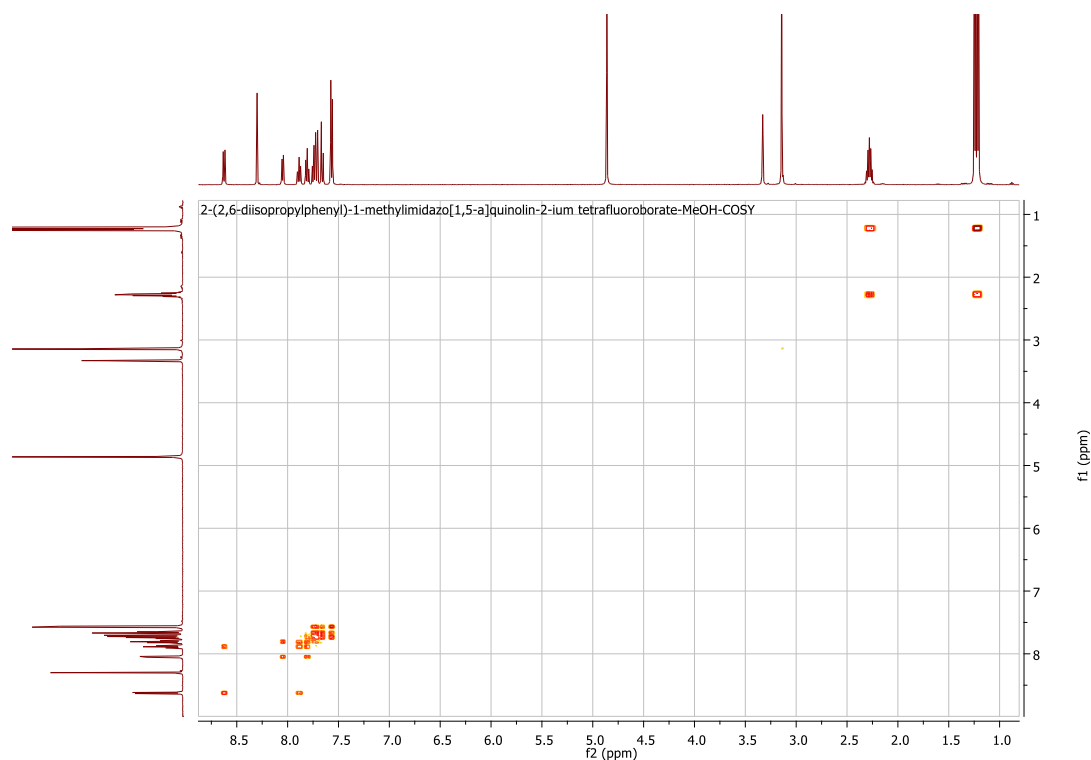


Figure S40. COSY-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol.

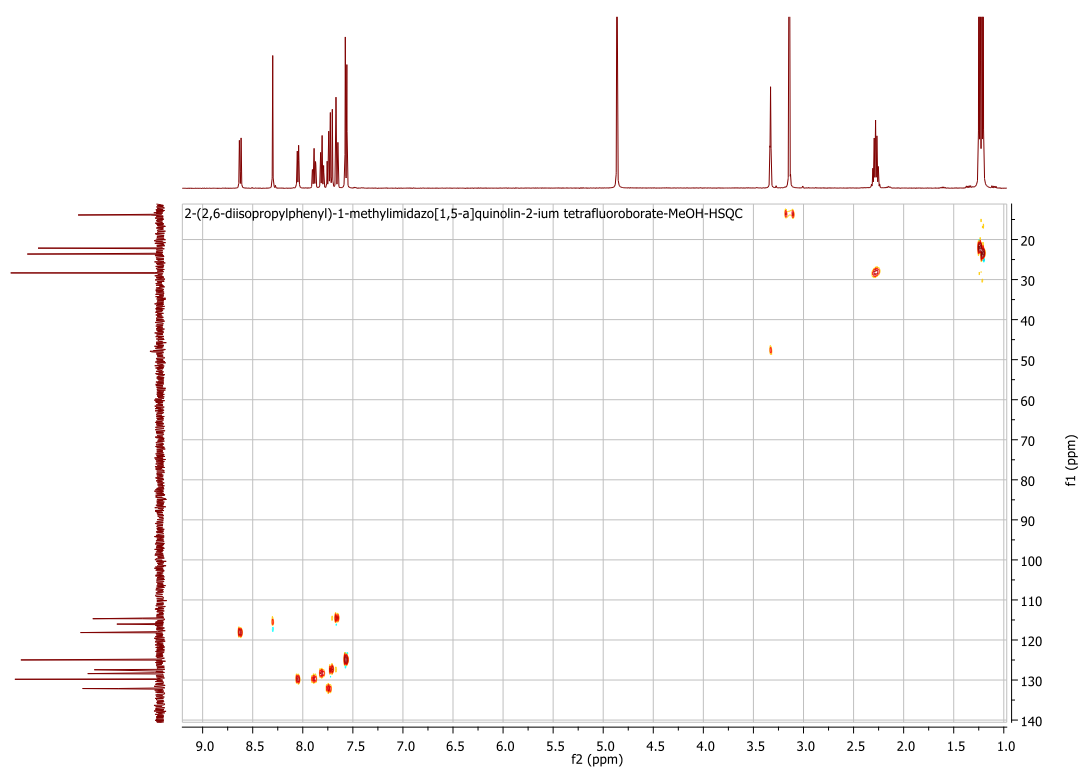


Figure S41. HSQC-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol.

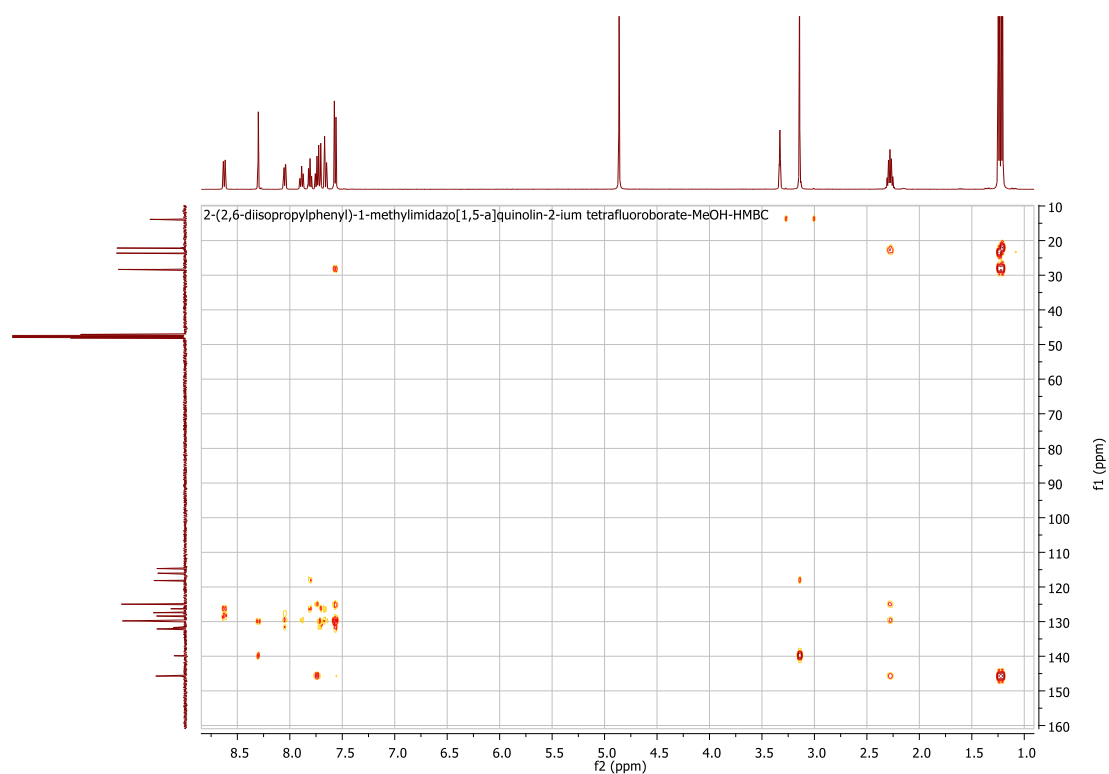
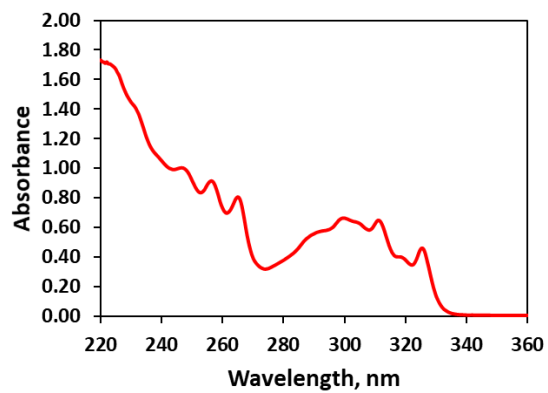
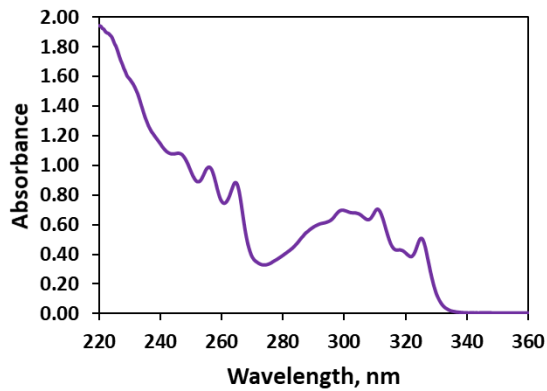


Figure S42. HMBC-NMR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in methanol.

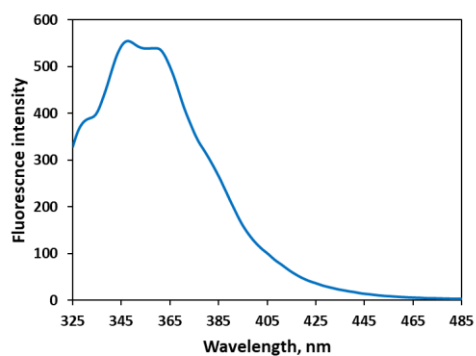


(a)

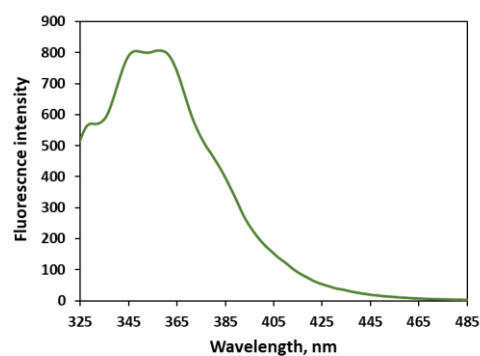


(b)

Figure S43. UV spectra of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** in (a) MeOH and (b) MeCN.

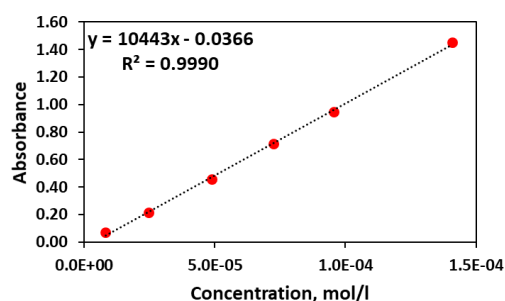


(a)

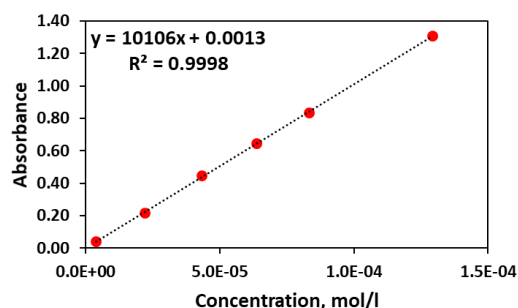


(b)

Figure S44. Fluorescent spectra of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetra-fluoroborate **1** in (a) MeOH, concentration 4.1×10^{-7} M and (b) MeCN, concentration 7.5×10^{-7} M. Excitation at 325 nm.



(a)



(b)

Figure S45. Calibration curves of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetra-fluoroborate – compound **1** in (a) MeOH and (b) MeCN. The dilutions are summarized in Table S1.

Table S1. Dilutions for the calibration curves. V_1 is the volume of the stock solution diluted to V_2 .

Solvent	Mass of compound 1 for the stock solution (g/10 mL)	V_1 (μL)	V_2 (μL)	Concentration (mol/l)	Absorbance
MeOH	0.01067	10	3000	$8.27\text{E-}06$	0.073
		30	3020	$2.46\text{E-}05$	0.214
		60	3050	$4.88\text{E-}05$	0.458
		90	3080	$7.25\text{E-}05$	0.716
		120	3110	$9.57\text{E-}05$	0.948
		180	3170	$1.41\text{E-}04$	1.451
MeCN	0.00482	10	3000	$3.73\text{E-}06$	0.040
		60	3050	$2.20\text{E-}05$	0.217
		120	3110	$4.32\text{E-}05$	0.447
		180	3170	$6.36\text{E-}05$	0.647
		240	3230	$8.32\text{E-}05$	0.835
		390	3380	$1.29\text{E-}04$	1.309

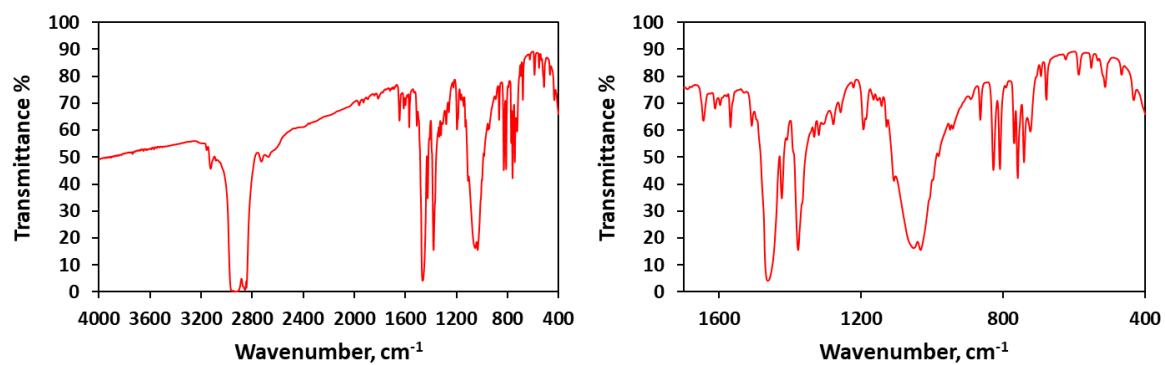


Figure S46. IR spectrum of 2-(2,6-diisopropylphenyl)-1-methylimidazo[1,5-a]quinolin-2-ium tetrafluoroborate **1** (nujol mull). For visual clarity the range 1700 – 400 cm⁻¹ is magnified (right image). Nujol absorbs in the range of 3000-2800 cm⁻¹ and at 1460 cm⁻¹ and 1380 cm⁻¹.