

Design, Synthesis, Photophysical and Electrochemical Properties of 2-(4,5-diphenyl-1-*p*-aryl-1H-imidazol-2-yl)phenol-based Boron Complexes

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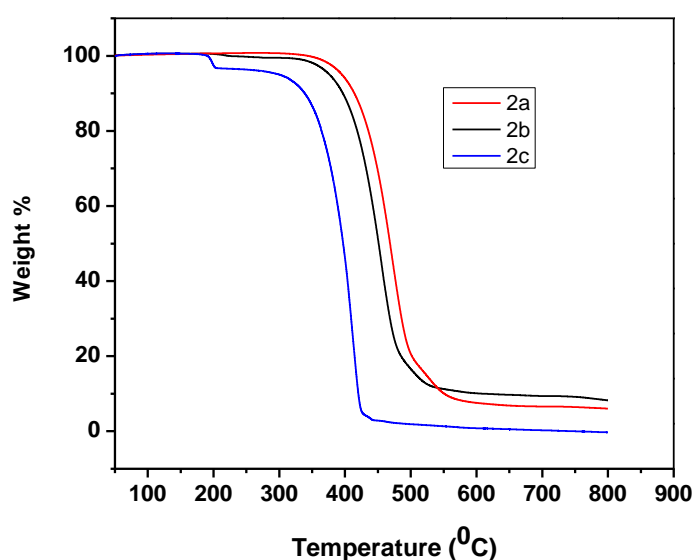


Figure S1. TGA curves of **2a-2c** at a heating rate of 20 °C/min

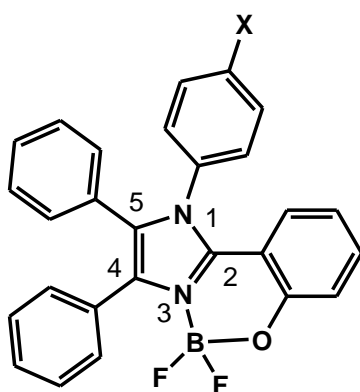
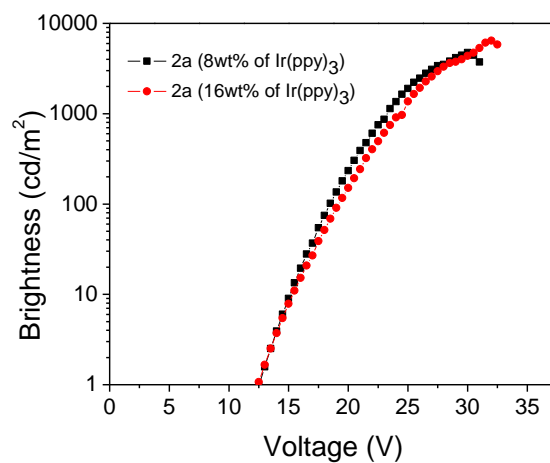


Figure S2. Imidazole core numbering used in the main text

(a)



(b)

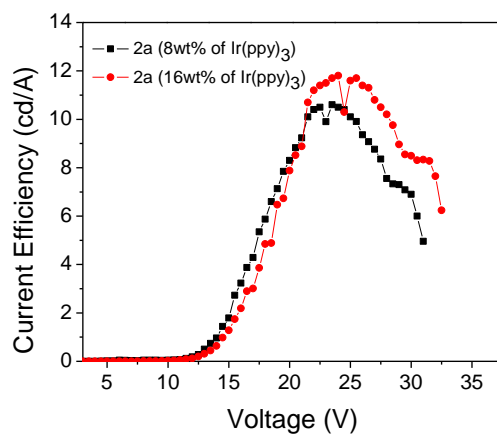


Figure S3. EL performances of device **2a** that contain different ratio of guest. (a) Brightness-Voltage, (b) Current Efficiency-Current Density.

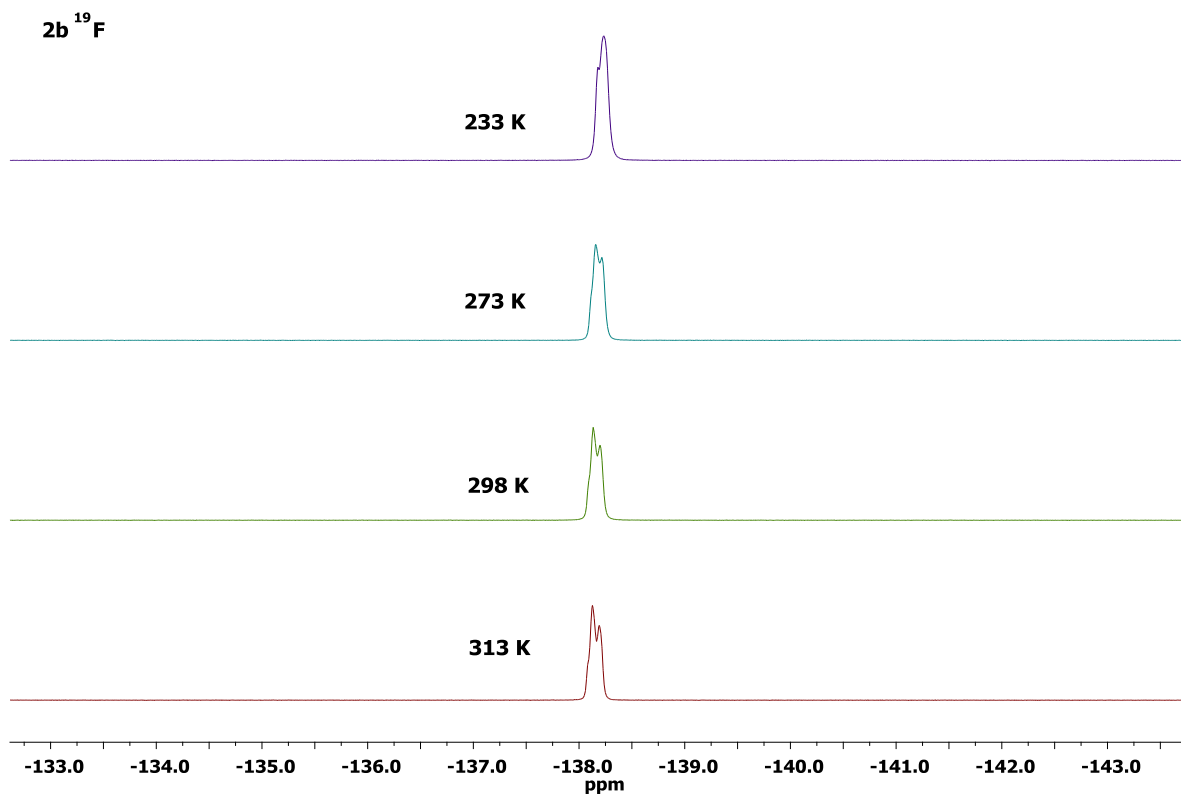


Figure S4. ¹⁹F variable temperature NMR (CDCl₃) of compound **2b**.

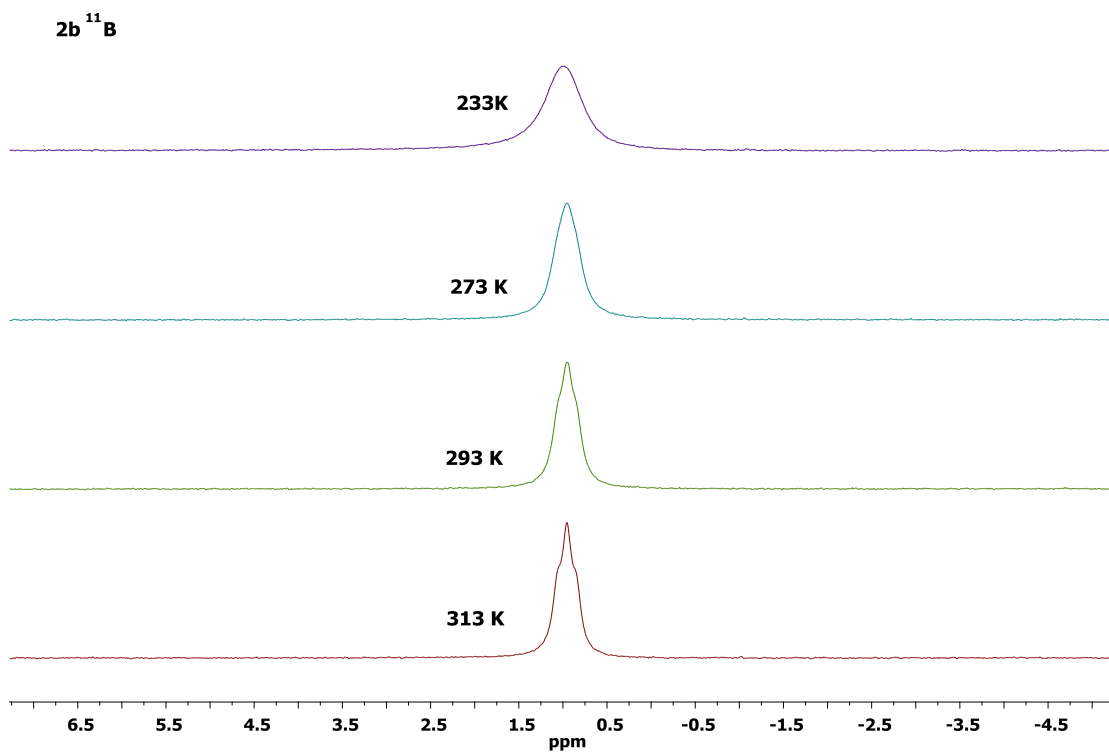


Figure S5. ¹¹B variable temperature NMR (CDCl₃) of compound **2b**.

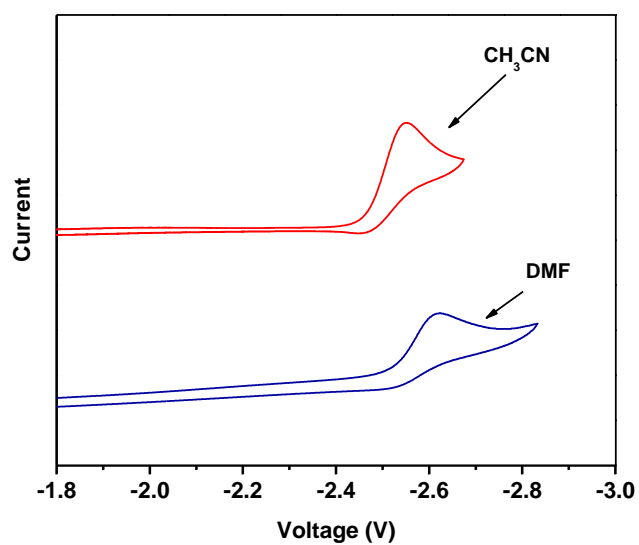


Figure S6. Cyclic voltammograms of compound **2a** (vs. Ferrocene/Ferrocenium) with 0.1 M Bu_4NPF_6 in DMF and CH_3CN as the supporting electrolyte (scan rate 100 mV/s).

Table S1. Electrochemical data of **2a-2c**

Compound	Solvent	$E_{\text{pa}}^{\#}$ (V)
2a	DMF	-2.62
	CH_3CN	-2.50
2b	DMF	-2.59
	CH_3CN	-2.61
2c	DMF	-2.43
	CH_3CN	-2.41

$^{\#}E_{\text{pa}}$ = anodic peak potential

Table S2. Calculated orbital energies (eV) for compound **2a-2c** from DFT (B3LYP) calculations

Compound	2a	2b	2c
LUMO+2	-0.897 (Im-1,2-Ph)	-0.8163 (Im-1,2-Ph)	-1.224 (Im-1,2-Ph)
LUMO+1	-1.006 (Im-1,4,5-Ph)	-0.952 (Im-1,4,5-Ph)	-1.360 (Im-1,2,5-Ph)
LUMO	-1.306 (Im-1,2,5-Ph)	-1.251 (Im-1,2,5-Ph)	-1.714 (Im-1,2 -Ph)
HOMO	-5.550 (Im-2,4-Ph, Oxygen)	-5.523 (Im-2,4-Ph, Oxygen)	-5.714 (Im-2,4-Ph, Oxygen)
HOMO-1	-6.095 (Im-2,4,5-Ph, Oxygen)	-6.067 (Im-2,4,5-Ph, Oxygen)	-6.231 (Im-2,4,5-Ph, Oxygen)
HOMO-2	-6.584 (4-Ph)	-6.557 (4-Ph)	-6.693 (4-Ph)

Table S3. Calculated electronic transitions for compound **2a-2c** from TD-DFT (B3LYP) calculations

Compound	Transition	MO contributions	Energy gap eV (nm)	Oscillator strength/f
2a	$S_0 \rightarrow S_1$	HOMO \rightarrow LUMO	3.74 (331)	0.2743
		HOMO \rightarrow LUMO+2		
	$S_0 \rightarrow S_2$	HOMO \rightarrow LUMO+1	3.97 (312)	0.0544
		HOMO \rightarrow LUMO+2		
	$S_0 \rightarrow S_3$	HOMO-1 \rightarrow LUMO	4.09 (303)	0.0788
		HOMO \rightarrow LUMO+1		
HOMO \rightarrow LUMO+2				
2b	$S_0 \rightarrow S_1$	HOMO \rightarrow LUMO	3.76 (329)	0.3137
	$S_0 \rightarrow S_2$	HOMO \rightarrow LUMO+1	4.00 (309)	0.0324
		HOMO \rightarrow LUMO+2		
	$S_0 \rightarrow S_3$	HOMO-1 \rightarrow LUMO	4.12 (300)	0.0683
		HOMO \rightarrow LUMO+1		
		HOMO \rightarrow LUMO+2		
2c	$S_0 \rightarrow S_1$	HOMO \rightarrow LUMO	3.42 (362)	0.0654
	$S_0 \rightarrow S_2$	HOMO-1 \rightarrow LUMO	3.80 (326)	0.0993
		HOMO \rightarrow LUMO+1		
		HOMO \rightarrow LUMO+2		
	$S_0 \rightarrow S_3$	HOMO-1 \rightarrow LUMO	3.93 (315)	0.1243
		HOMO \rightarrow LUMO+2		

Table S4. Computed orbitals for compounds **2a-2c**



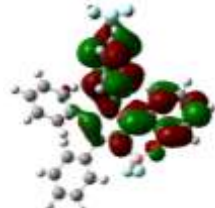
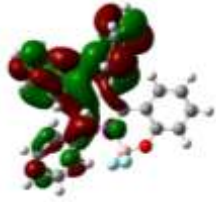
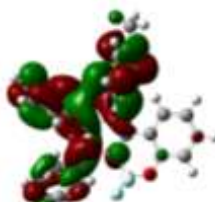






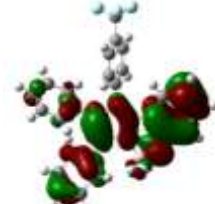
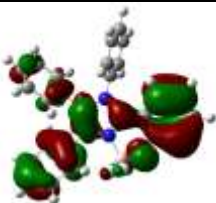


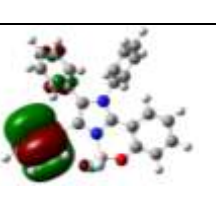
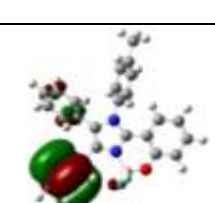
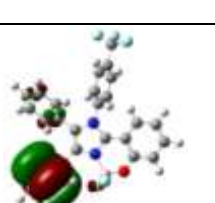
Compound	2a	2b	2c
LUMO+2			
LUMO+1			
LUMO			
HOMO			
HOMO-1			
HOMO-2			

Table S5. Details of X-ray crystal structure analyses of compound **2a** and **2c**.

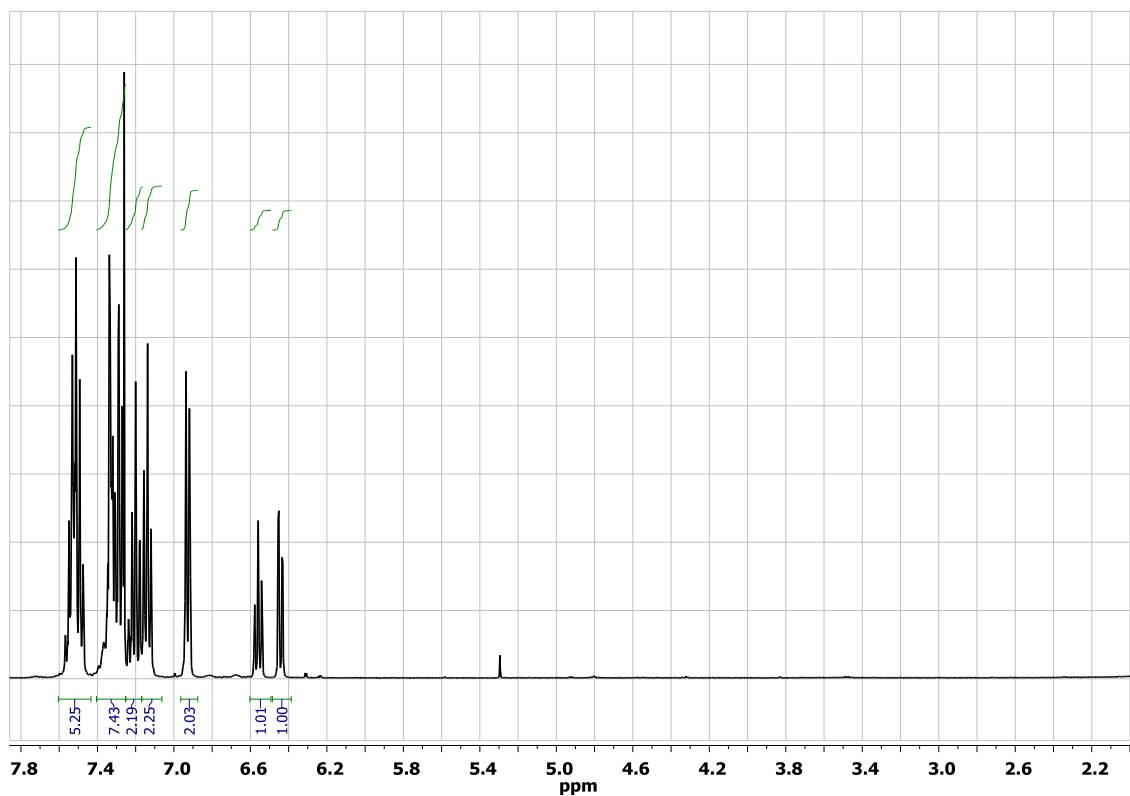
	2a	2c.CH₃CN
formula	C ₂₇ H ₁₉ BF ₂ N ₂ O	C ₅₈ H ₃₆ B ₂ F ₁₀ N ₅ O ₂
M _r	436.25	1046.54
T [K]	296(2)	100(2)
wavelength, Å	0.71073 Å	0.71073 Å
crystal system	Triclinic	Monoclinic
space group	<i>P</i> -1	<i>C</i> 2/ <i>c</i>
a [Å]	10.2847(4)	31.603(4)
b [Å]	10.8082(4)	8.6107(10)
c [Å]	10.9755(4)	22.928(3)
α [°]	85.101(3)	90
β [°]	75.591(3)	129.760(11)
δ [°]	67.342(2)	90
V [Å ³]	1090.38(7)	4796.3(11)
Z	2	4
ρ _{calc} [g cm ⁻³]	1.329	1.449
μ (MoKα) [mm ⁻¹]	0.092	0.115
F (000)	452	2140
Crystal size [mm]	0.25 x 0.22 x 0.20	0.40 x 0.35 x 0.30
θ range [°]	1.92 – 28.30	1.68 – 30.56
limiting indices	-12 ≤ h ≤ 13 -14 ≤ k ≤ 14 -14 ≤ l ≤ 14	-45 ≤ h ≤ 44 -12 ≤ k ≤ 12 -31 ≤ l ≤ 32
reflns collected	16890	39509
independent reflns	5404	7309
absorption correction	[R(int) = 0.0375] Semi-empirical from equivalents	[R(int) = 0.0307] Semi-empirical from equivalents
refinement method	Full-matrix least square on F ²	Full-matrix least square on F ²
data / restraints / parameters	5404 / 0 / 299	7309 / 0 / 349
Goodness-of-fit on F ²	1.006	1.033
final R indices	R ₁ = 0.0465	R ₁ = 0.0414
[I > 2σ(I)] [a]	wR ₂ = 0.1059	wR ₂ = 0.1122
R indices (all data) [a]	R ₁ = 0.0945	R ₁ = 0.0499
	wR ₂ = 0.1302	wR ₂ = 0.1187
peak _{max} /hole _{min} [e Å ⁻³]	0.200 and -0.142	0.607 and -0.316

[a] $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; $wR_2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]\}^{1/2}$.

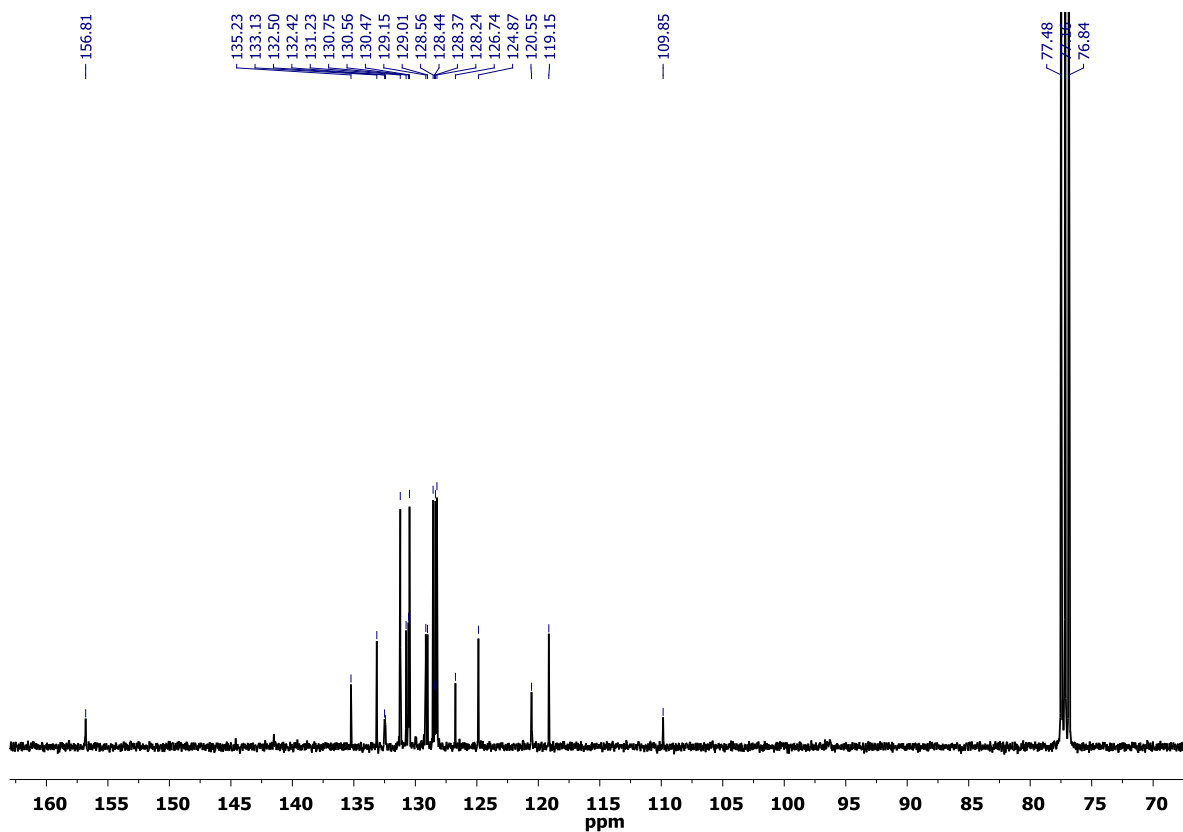
Table S6. EL characters of the device **2a** that contain different ratio of guest.

Device	Turn-on voltage at 1cd/m ² (V)	Max. brightness (cd/m ²)	Efficiency (cd/A)/voltage(v)
2a (8 wt% of Ir(ppy) ₃)	12.5	4760	10.6
2a (16 wt% of Ir(ppy) ₃)	12.5	6450	11.8

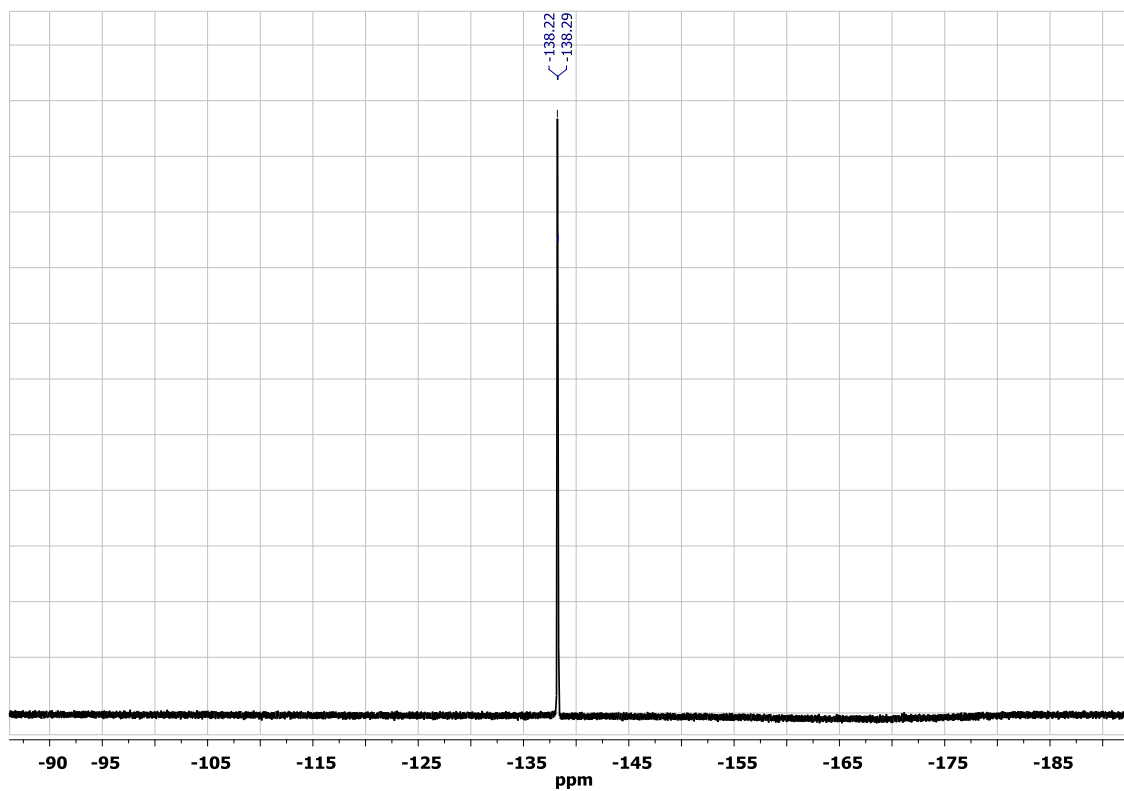
Compound 2a ¹H NMR



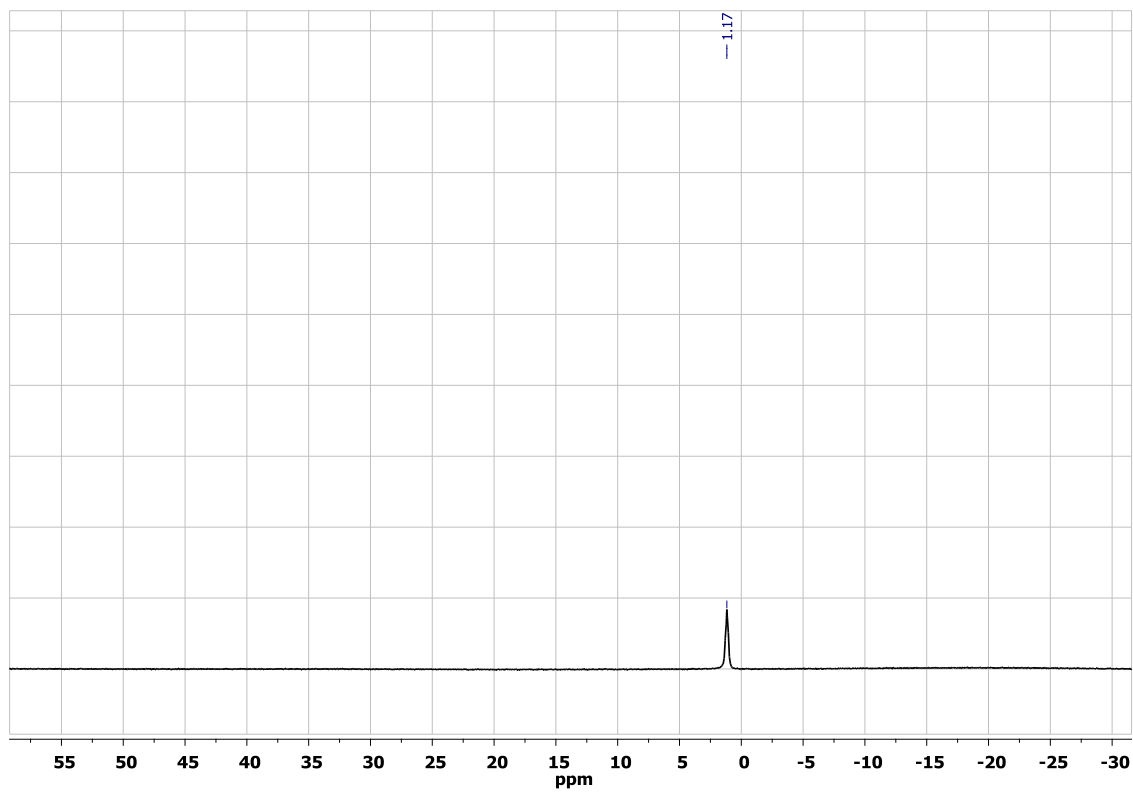
Compound 2a ¹³C NMR



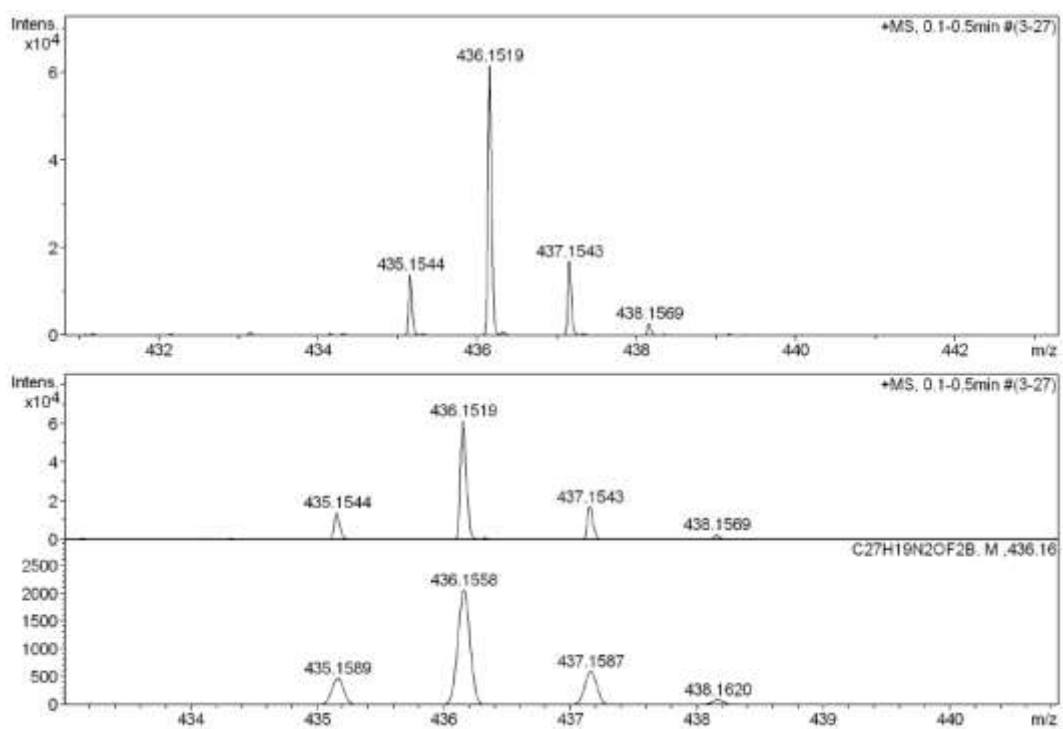
Compound 2a ^{19}F NMR



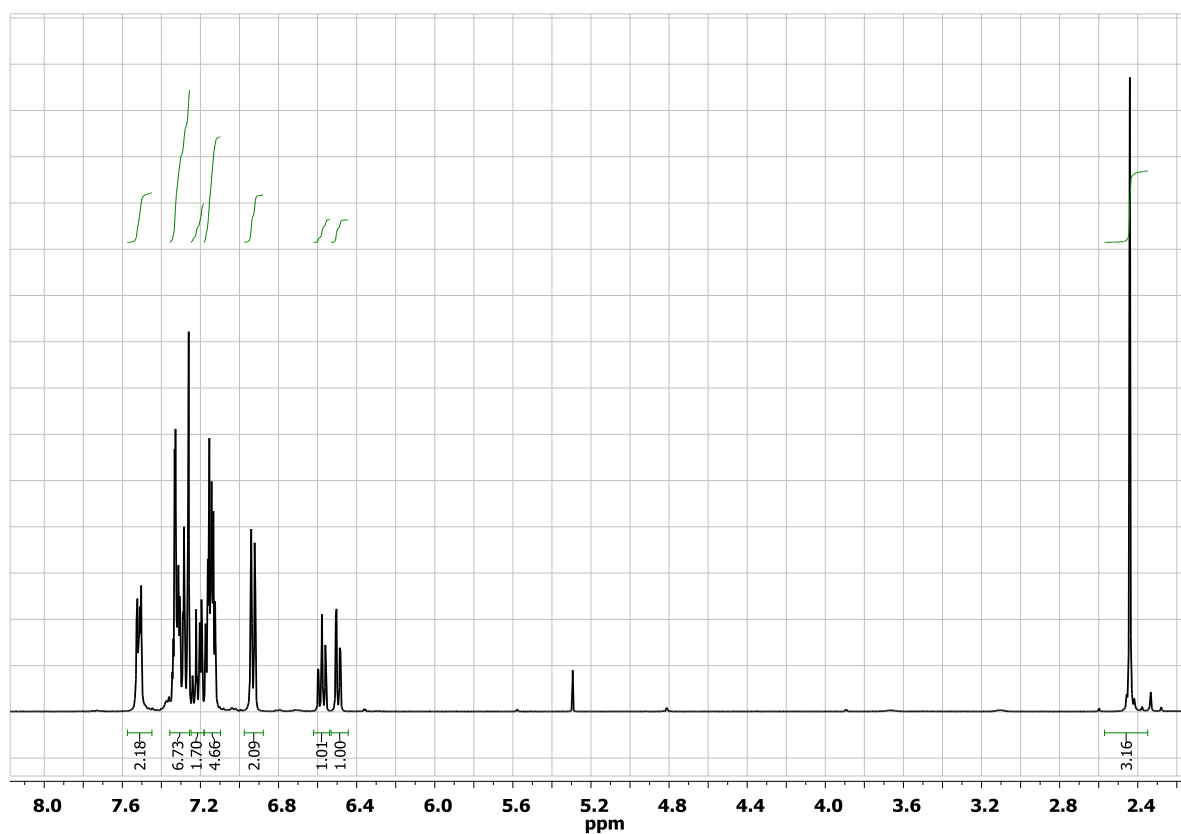
Compound 2a ^{11}B NMR



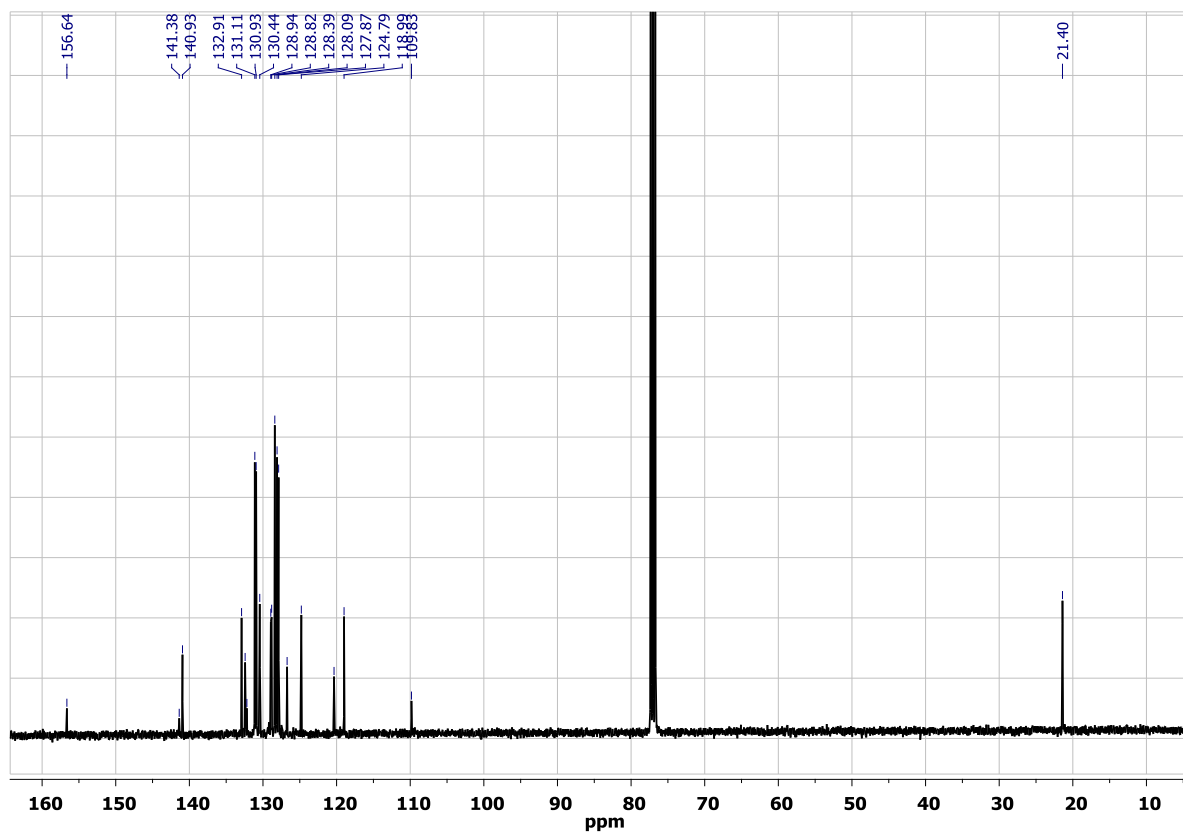
Compound 2a HRMS



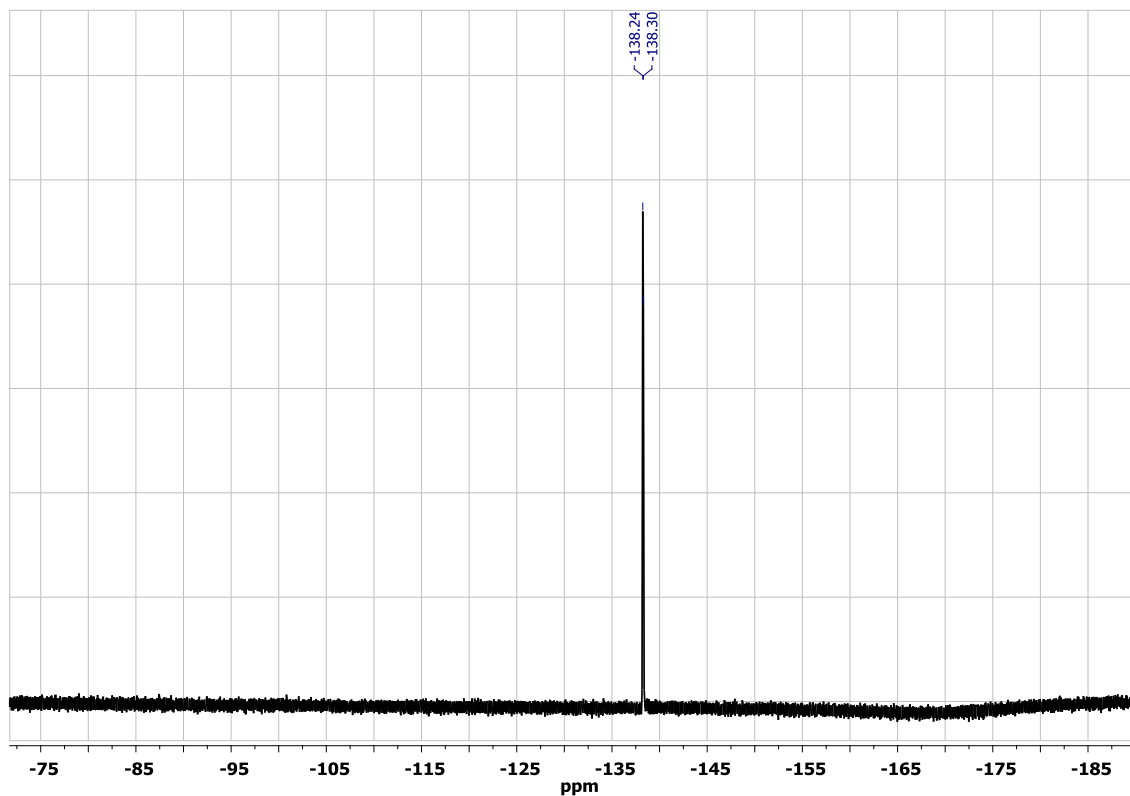
Compound 2b ¹H NMR



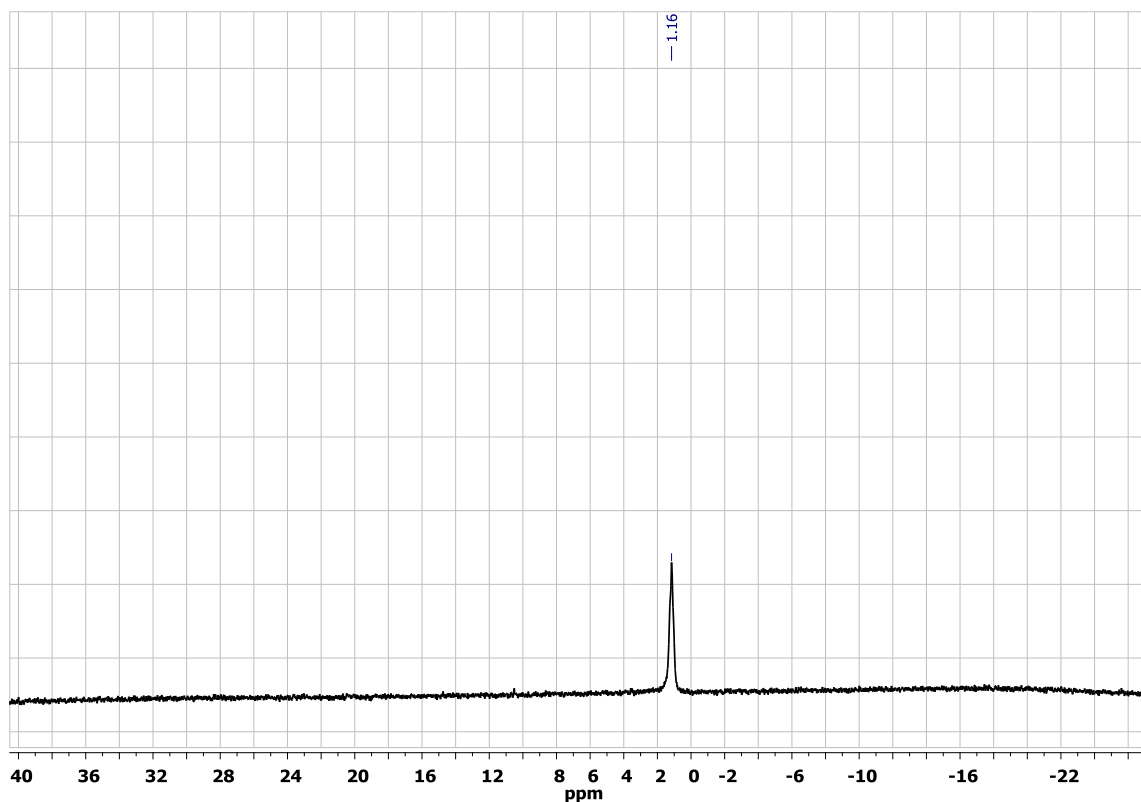
Compound **2b** ^{13}C NMR



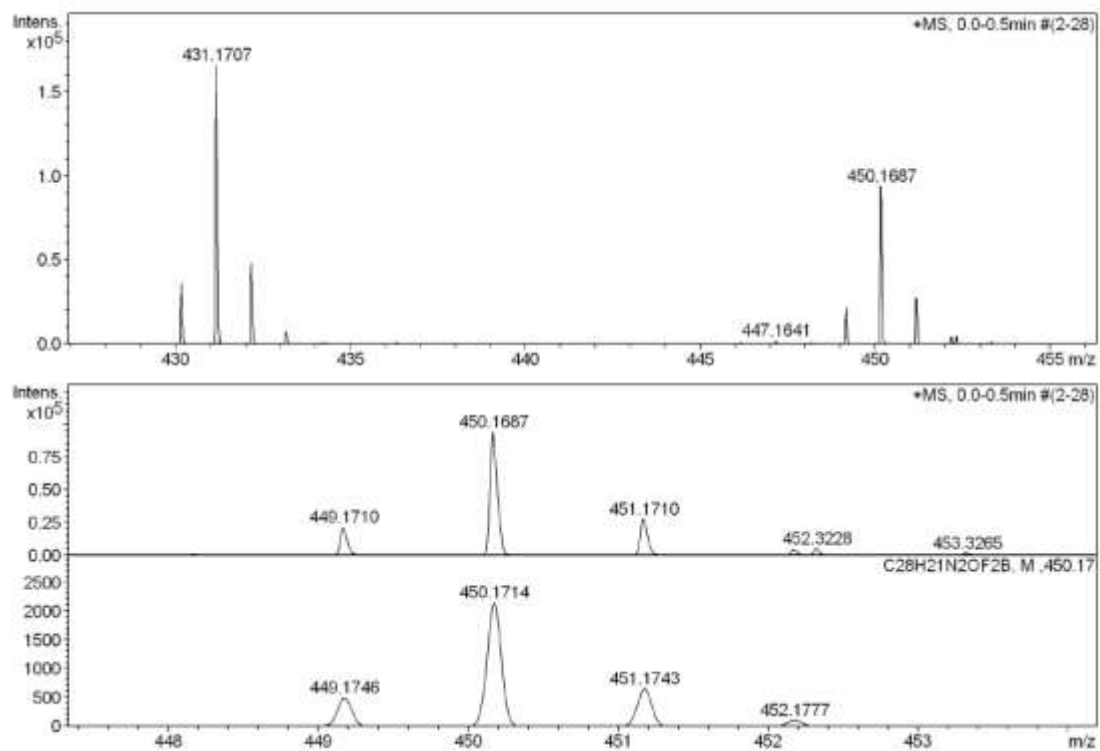
Compound **2b** ^{19}F NMR



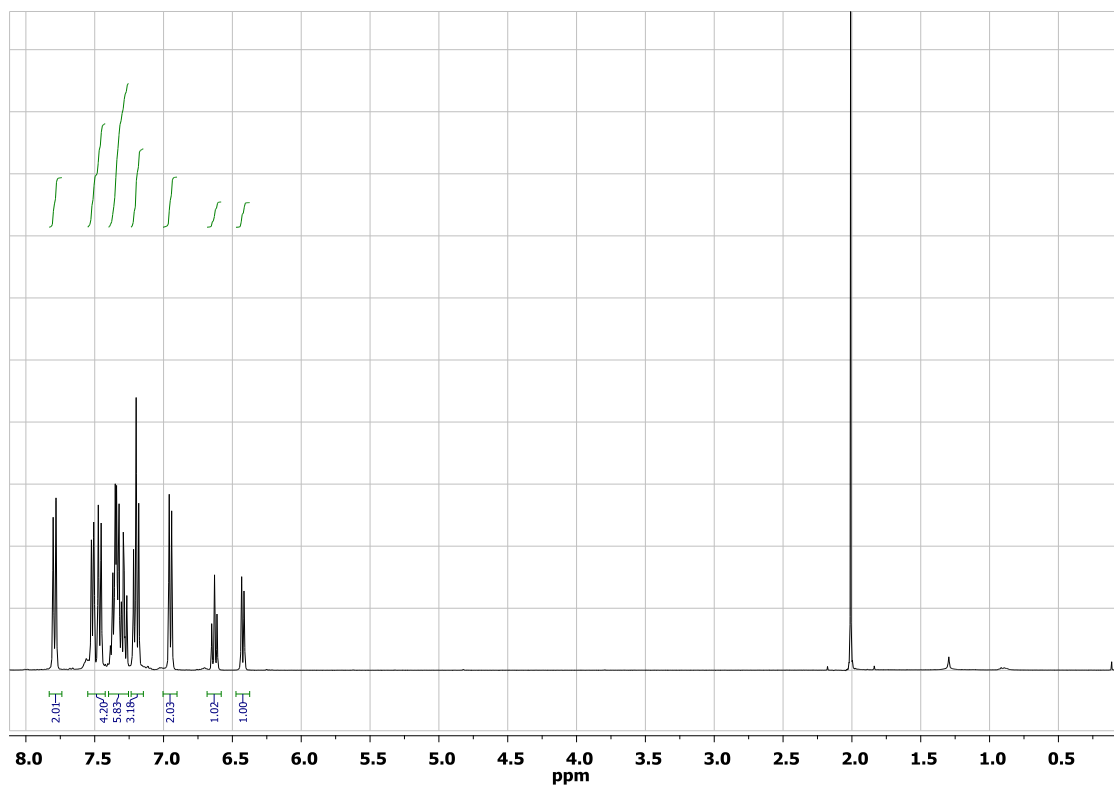
Compound **2b** ^{11}B NMR



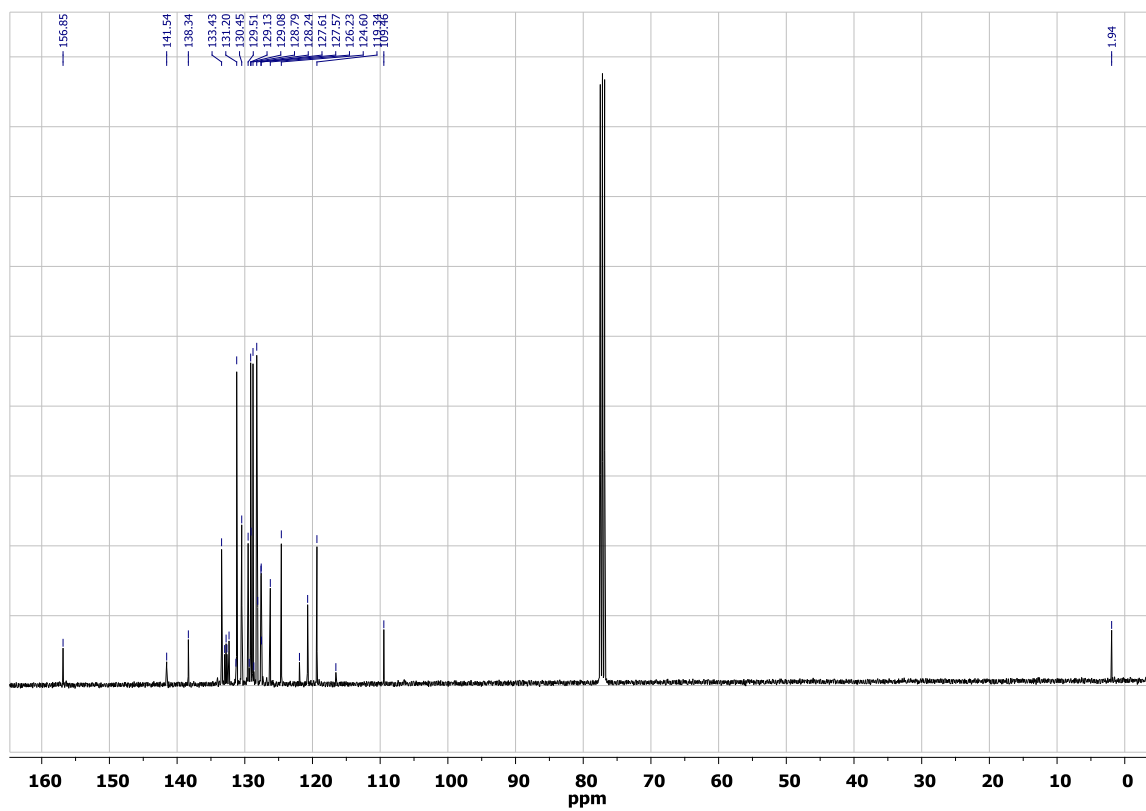
Compound **2b** HRMS



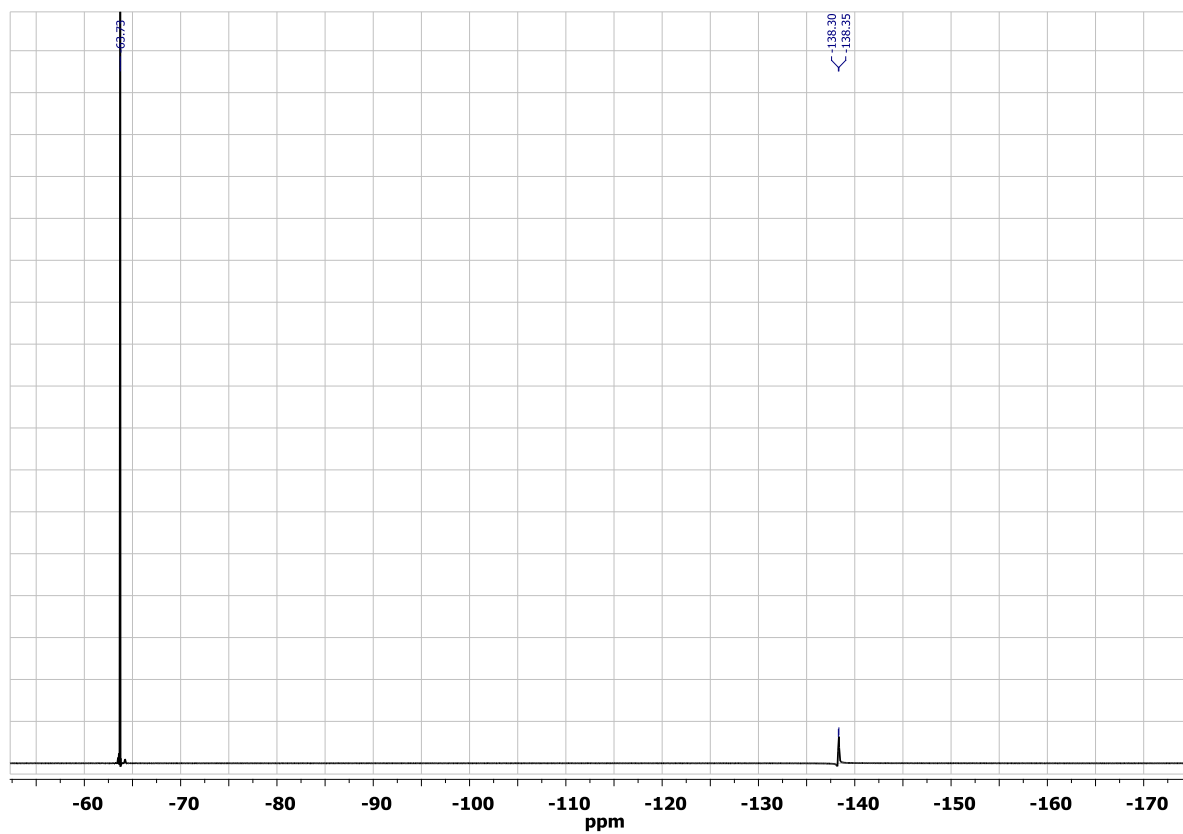
Compound 2c ^1H NMR



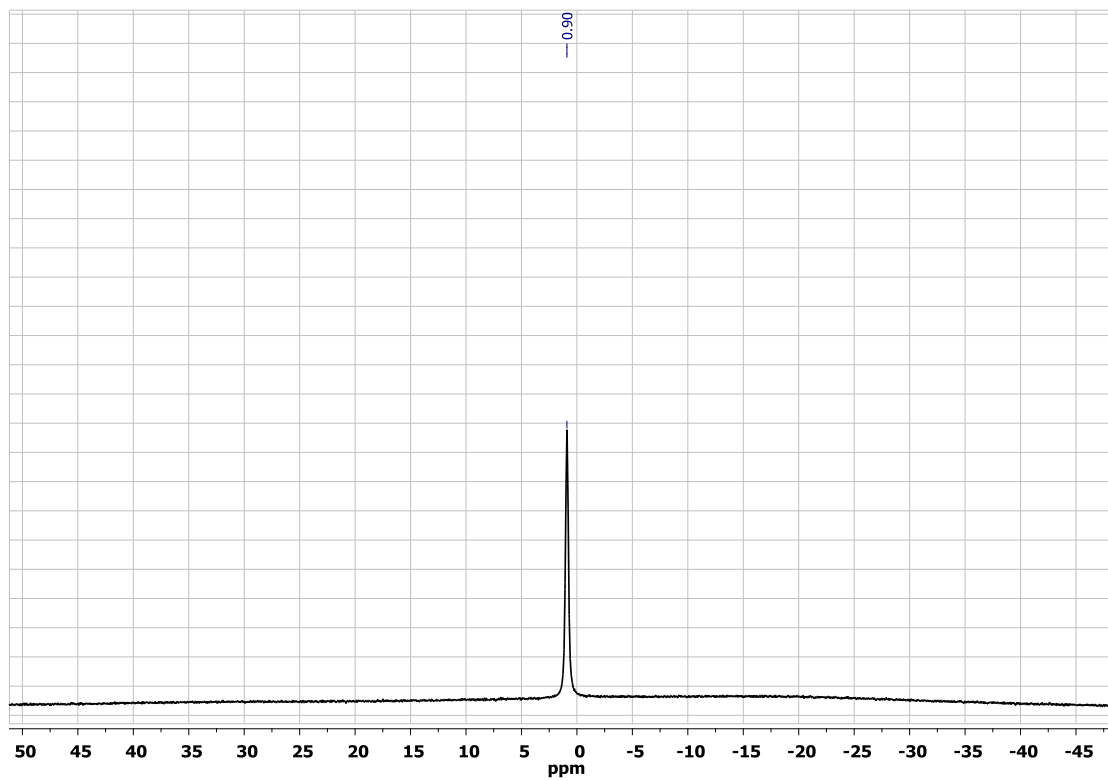
Compound 2c ^{13}C NMR



Compound **2c** ^{19}F NMR



Compound **2c** ^{11}B NMR



Compound 2c HRMS

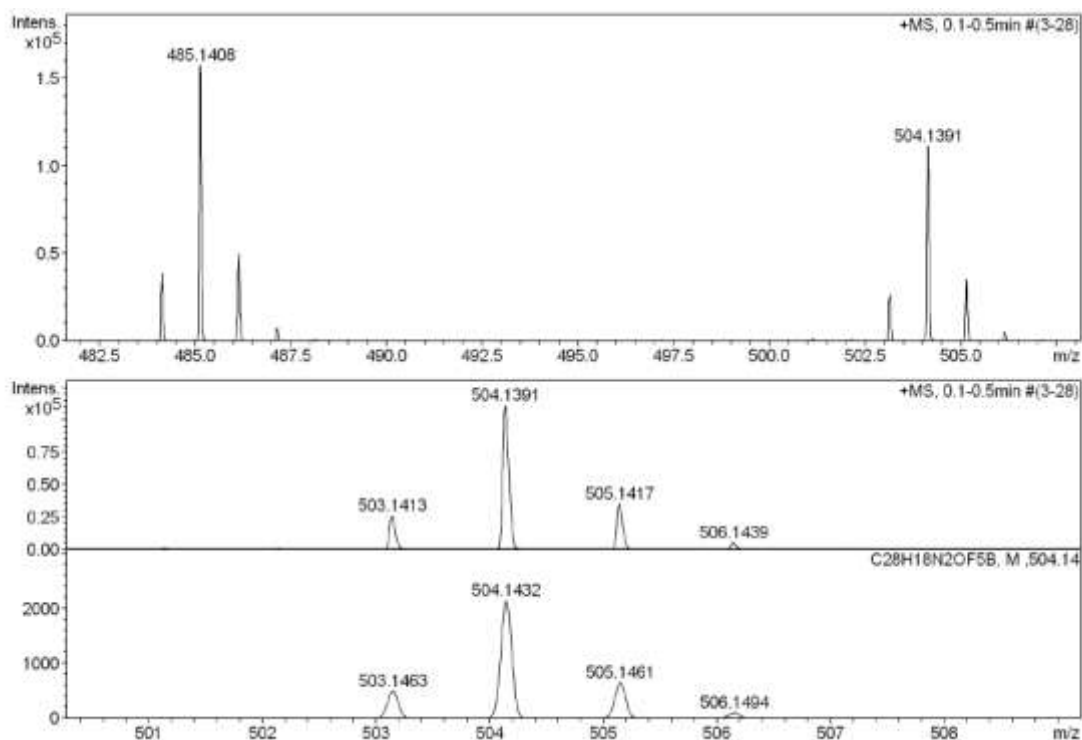


Table S7

Optimized x,y,z coordinates for compounds **2a-2c**, calculated on Gaussian 03 at the B3LYP//6-31g(d) level

Compound 2a

F	0.297435	-3.489323	1.224358
F	-0.411815	-3.566801	-0.965443
O	1.827535	-3.147522	-0.534541
N	0.618407	0.733544	0.030812
N	0.159012	-1.412663	-0.004627
C	-4.917356	-2.583216	-0.133980
H	-5.901776	-3.043326	-0.153913
C	-4.626582	-1.513015	-0.981522
H	-5.380757	-1.138159	-1.668297
C	-3.362911	-0.925976	-0.958112
H	-3.137467	-0.101339	-1.627132
C	-2.371914	-1.401602	-0.084697
C	-1.053576	-0.738369	-0.037428
C	-0.781865	0.612066	-0.011074
C	1.330693	1.981736	0.004826
C	1.331955	2.800373	1.135299
H	0.803194	2.483694	2.028543

C	2.015936	4.015983	1.098408
H	2.020141	4.655880	1.975898
C	1.997449	2.367905	-1.160409
H	1.984482	1.714931	-2.027656
C	2.683494	3.581807	-1.186313
H	3.208554	3.882669	-2.088150
C	2.802694	-2.297525	-0.230163
C	2.550644	-0.936784	0.102310
C	3.635061	-0.104181	0.448730
H	3.455108	0.917948	0.755714
C	4.936438	-0.582619	0.422492
H	5.757912	0.071078	0.699227
C	5.181304	-1.910459	0.042615
H	6.200463	-2.287189	0.013873
C	4.130758	-2.756542	-0.277127
H	4.294663	-3.793168	-0.552588
C	1.159943	-0.522102	0.050775
C	-3.934376	-3.066005	0.732047
H	-4.149874	-3.905043	1.387909
C	-2.669172	-2.483072	0.760421
H	-1.902877	-2.874265	1.419929
C	-1.699018	1.767725	0.035743
C	-1.633434	2.802902	-0.911494
H	-0.891451	2.762914	-1.702738
C	-2.521041	3.876340	-0.849603
H	-2.458522	4.668164	-1.591056
C	-3.490926	3.929620	0.153015
H	-4.183727	4.765477	0.197913
C	-3.568906	2.902478	1.095660
H	-4.321560	2.935591	1.878534
C	-2.679228	1.831111	1.040322
H	-2.739933	1.032798	1.773489
B	0.449512	-2.997869	-0.065399
C	2.693238	4.406111	-0.058682
H	3.227280	5.351682	-0.082075

Compound 2b

F	2.004625	3.106684	1.220271
F	2.623182	2.760793	-0.971037
O	0.557638	3.719808	-0.535036
N	-0.711812	-0.142822	0.031302
N	0.908986	1.337503	-0.008826
C	5.720260	-0.663701	-0.141579
H	6.788553	-0.862557	-0.162379
C	4.858441	-1.374946	-0.978045
H	5.251577	-2.126788	-1.657124
C	3.489301	-1.116594	-0.953539
H	2.823957	-1.663766	-1.613963
C	2.962499	-0.143042	-0.089745
C	1.504437	0.084145	-0.040545

C	0.498249	-0.856818	-0.011469
C	-2.016560	-0.745497	0.011599
C	-2.497105	-1.402825	1.144120
H	-1.886819	-1.448187	2.040481
C	-3.761643	-1.988816	1.112639
H	-4.133492	-2.496098	1.999216
C	-4.561712	-1.931423	-0.036628
C	-5.920504	-2.589953	-0.070878
C	-2.791822	-0.680622	-1.147789
H	-2.410659	-0.160863	-2.021560
C	-4.056168	-1.265470	-1.162317
H	-4.660034	-1.202336	-2.064045
C	-0.729555	3.593817	-0.228983
C	-1.314319	2.339216	0.102040
C	-2.680561	2.291281	0.448836
H	-3.128107	1.354103	0.752905
C	-3.461609	3.437014	0.425883
H	-4.509844	3.381565	0.703231
C	-2.889791	4.660877	0.048503
H	-3.500217	5.559863	0.022325
C	-1.543432	4.739371	-0.272344
H	-1.074478	5.678692	-0.546402
C	-0.423200	1.193521	0.049134
C	5.204328	0.311155	0.714461
H	5.869814	0.875793	1.361706
C	3.836230	0.573422	0.744303
H	3.442619	1.344250	1.396916
C	0.573369	-2.330205	0.039306
C	-0.077916	-3.137605	-0.907820
H	-0.656836	-2.676366	-1.701782
C	0.022255	-4.526792	-0.842160
H	-0.485452	-5.137247	-1.583992
C	0.777907	-5.130622	0.164442
H	0.857193	-6.213276	0.212018
C	1.434043	-4.336988	1.107362
H	2.025337	-4.798651	1.893330
C	1.331093	-2.948391	1.048155
H	1.841660	-2.332014	1.781610
B	1.592650	2.796400	-0.069404
H	-6.609405	-2.053369	-0.731371
H	-5.849537	-3.620810	-0.442330
H	-6.369762	-2.633503	0.926432

Compound 2c

F	-6.375314	0.442236	-0.777715
F	-6.309274	-0.550837	1.162290
F	-6.055759	-1.703028	-0.663572
F	3.554792	2.376915	1.181540
F	3.998263	1.821889	-1.009718
O	2.354844	3.397604	-0.571515
N	-0.078923	0.160371	0.065069

N	1.932478	1.035313	-0.007086
C	5.839621	-2.406057	-0.179011
H	6.787506	-2.936742	-0.210173
C	4.783462	-2.809334	-0.997647
H	4.905364	-3.651895	-1.672973
C	3.569547	-2.126016	-0.960238
H	2.755186	-2.435413	-1.607758
C	3.395565	-1.029134	-0.101355
C	2.089570	-0.343865	-0.037753
C	0.834629	-0.909395	0.011655
C	-1.505721	0.012489	0.045887
C	-2.161122	-0.526327	1.154027
H	-1.590393	-0.815091	2.030105
C	-3.545006	-0.687196	1.122931
H	-4.062863	-1.100487	1.981364
C	-4.266658	-0.304442	-0.009762
C	-5.756434	-0.526027	-0.068597
C	-2.222214	0.389934	-1.093162
H	-1.697234	0.811602	-1.944122
C	-3.605453	0.236273	-1.116610
H	-4.170639	0.538849	-1.991715
C	1.106083	3.699302	-0.232088
C	0.157284	2.703561	0.133935
C	-1.137827	3.101674	0.525589
H	-1.851845	2.362722	0.866494
C	-1.507915	4.437712	0.505718
H	-2.506656	4.726604	0.818072
C	-0.584858	5.407949	0.087413
H	-0.873494	6.455475	0.063074
C	0.703582	5.045714	-0.273775
H	1.440820	5.781815	-0.576924
C	0.628226	1.332249	0.070681
C	5.675641	-1.311909	0.672585
H	6.496058	-0.986115	1.306019
C	4.464309	-0.624879	0.715125
H	4.348107	0.235696	1.364010
C	0.425793	-2.326895	0.064033
C	-0.449859	-2.878215	-0.886040
H	-0.839645	-2.255502	-1.685529
C	-0.812271	-4.222878	-0.818399
H	-1.489151	-4.634729	-1.561812
C	-0.301267	-5.038131	0.193110
H	-0.582619	-6.086383	0.242712
C	0.575418	-4.501685	1.138247
H	0.978979	-5.129994	1.927375
C	0.934751	-3.156400	1.077260
H	1.616558	-2.740004	1.812392
B	3.049345	2.199203	-0.098473