Supporting Information

New AIE-active Pyrimidine-Based Boronfluoride Complexes with High Solid-State Emission and Reversible Mechanochromism Luminescence Behavior

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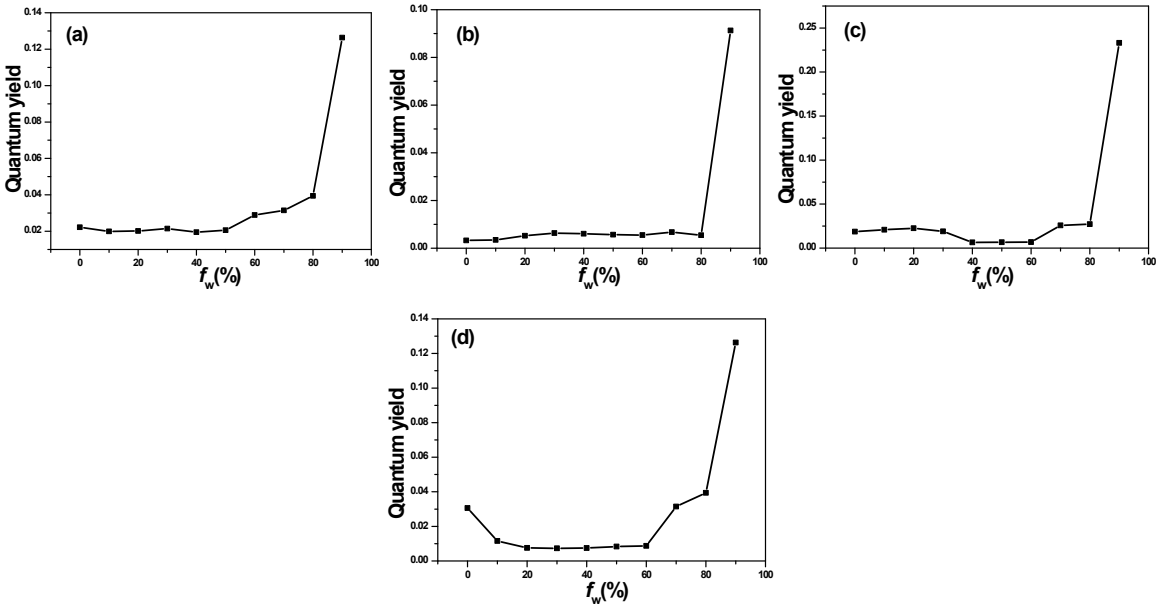


Figure S1. Changes in the quantum yields of compounds **PB-1** (a), **PB-2** (b), **PB-3** (c) and **PB-4**(d) in water/THF mixtures with varied volumetric fractions of water (f_w).

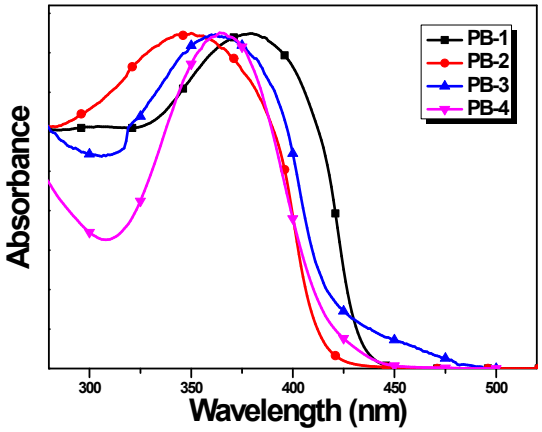


Figure S2. Absorption of **PB-1–4** in drop-cast film.

Table S1. Calculated excited wavelength (λ) and oscillator strengths (*f*) and related wave functions.

Compound	State[a]	Energy [eV]	λ [nm]	*f*[b]	Orbitals (coefficient) [c]
PB-1	S1	3.8136	325.11	0.5925	H>L (95%)
	S2	4.5915	270.00	0.0904	H>L+1 (84%)
PB-2	S1	4.0244	308.08	0.6623	H>L (95%)
	S2	4.6374	267.36	0.0317	H-3>L+1 (2%), H>L+1 (88%)
PB-3	S1	4.1037	302.13	0.6960	H>L (95%)
	S2	4.8592	255.15	0.0010	H-3>L+1 (2%), H-1>L (13%), H>L+1 (76%)
PB-4	S1	3.9711	312.21	0.9708	H>L (92%)
	S2	4.6787	265.00	0.0051	H-9>L (2%), H-1>L (60%), H>L+1 (29%)

[a] Excited state; [b] Oscillator strength; [c] MOs involved in the transitions, H = HOMO, L = LUMO.

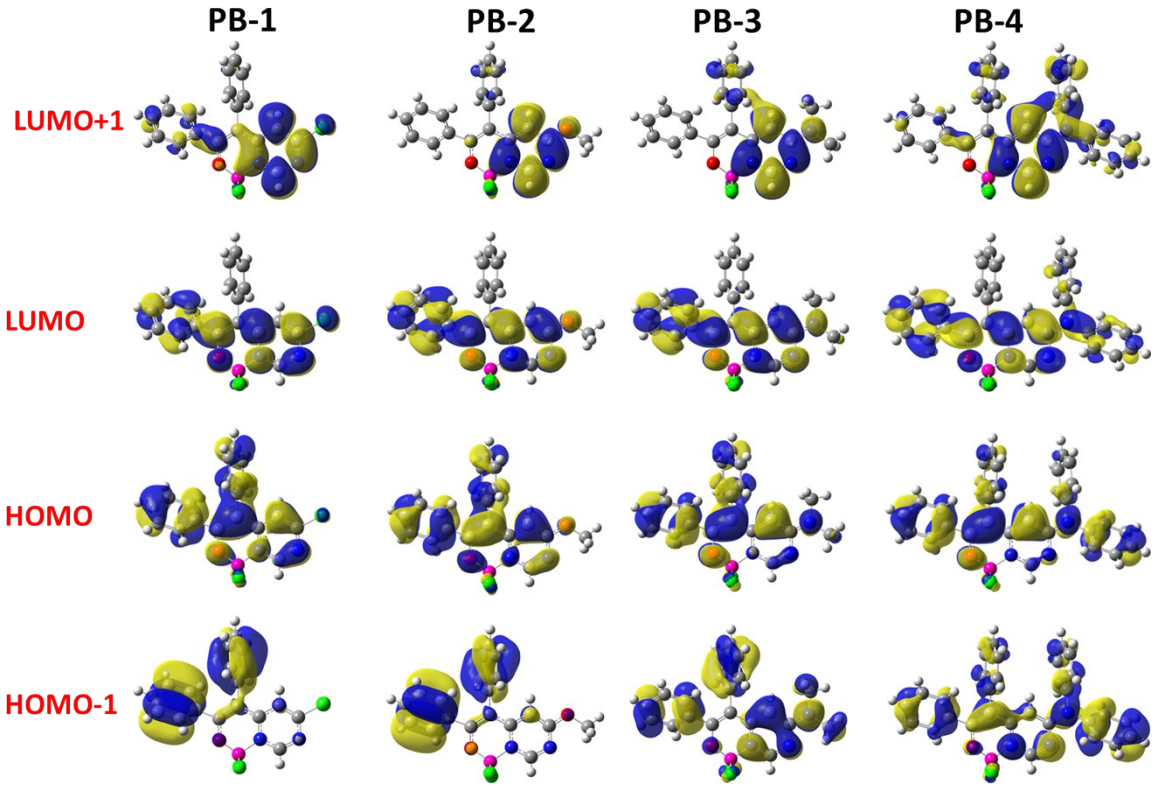


Figure S3. Molecular orbital amplitude plots of **PB-1–4** calculated by using CAM-B3LYP/6-31+G(d) basis set with G03 program.

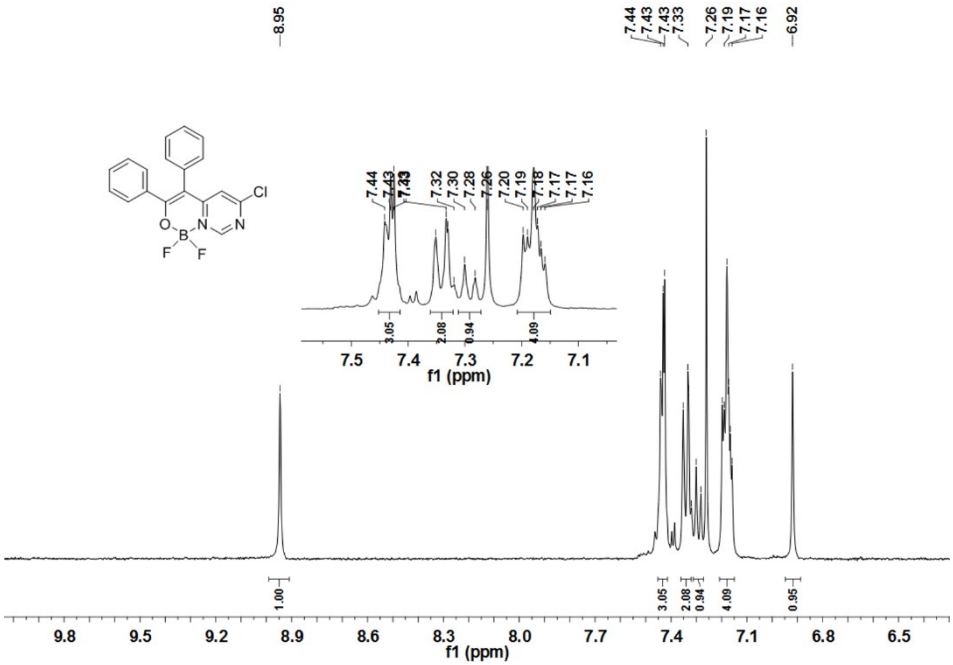


Figure S4. ^{1}H NMR of **PB-1** in $CDCl_3$.

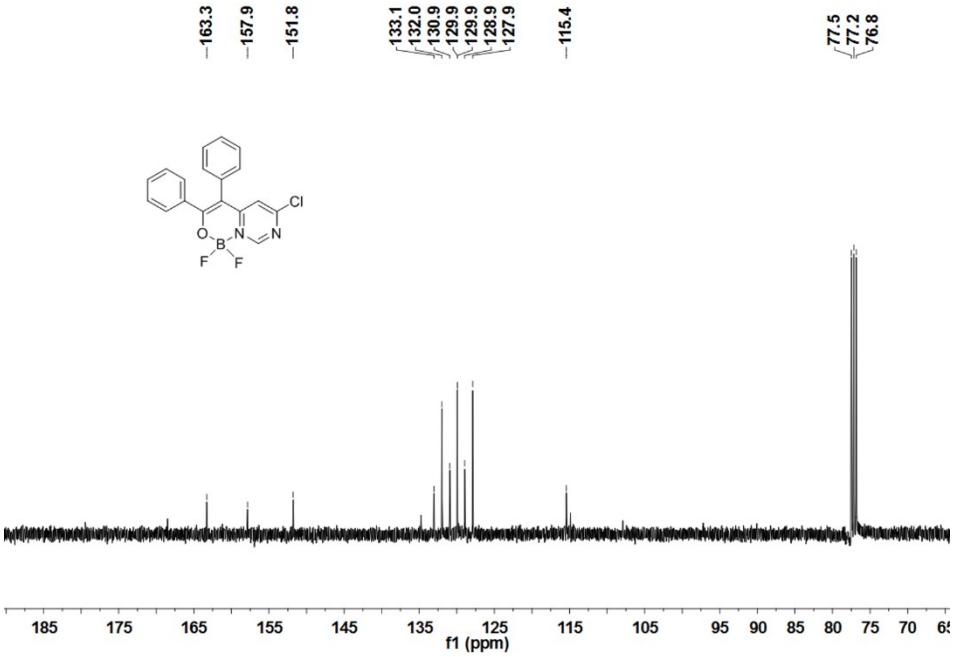


Figure S5. ^{13}C NMR of **PB-1** in $CDCl_3$.

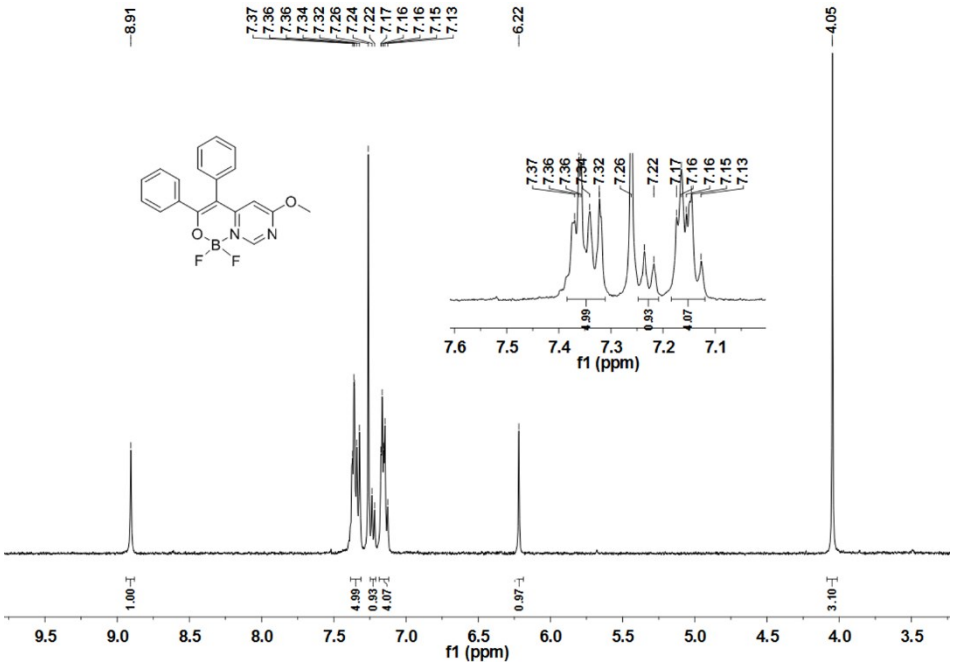


Figure S6. ^{1}H NMR of **PB-2** in $CDCl_3$.

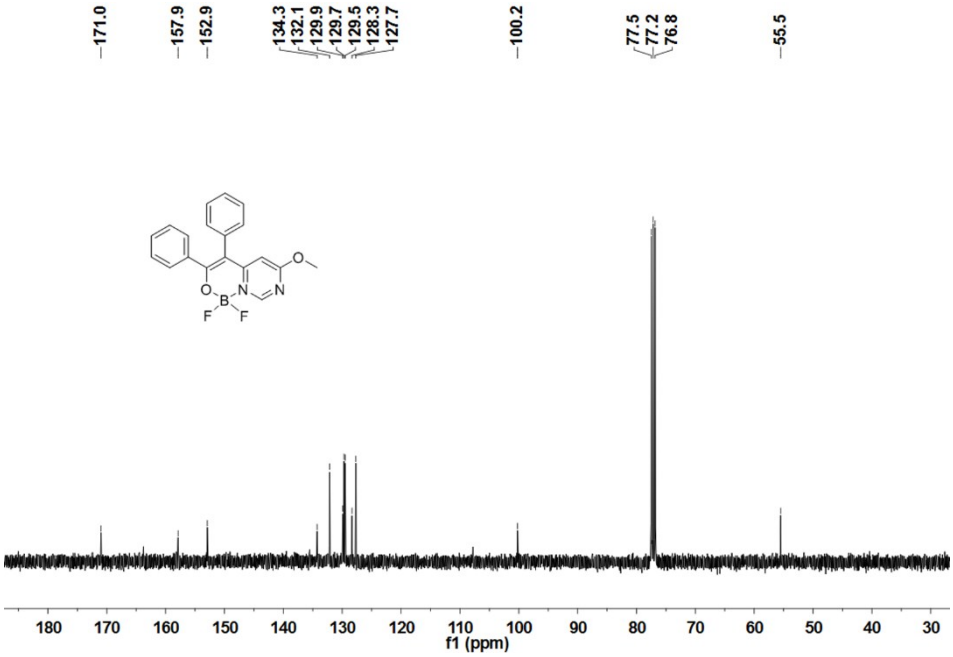


Figure S7. ^{13}C NMR of **PB-2** in $CDCl_3$.

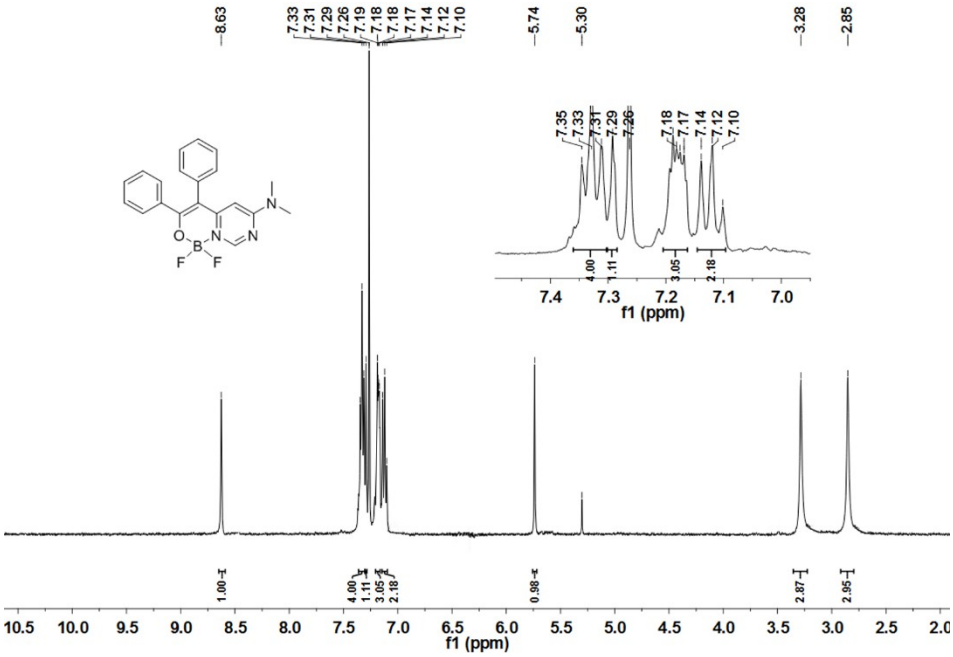


Figure S8. ^{1}H NMR of **PB-3** in $CDCl_3$.

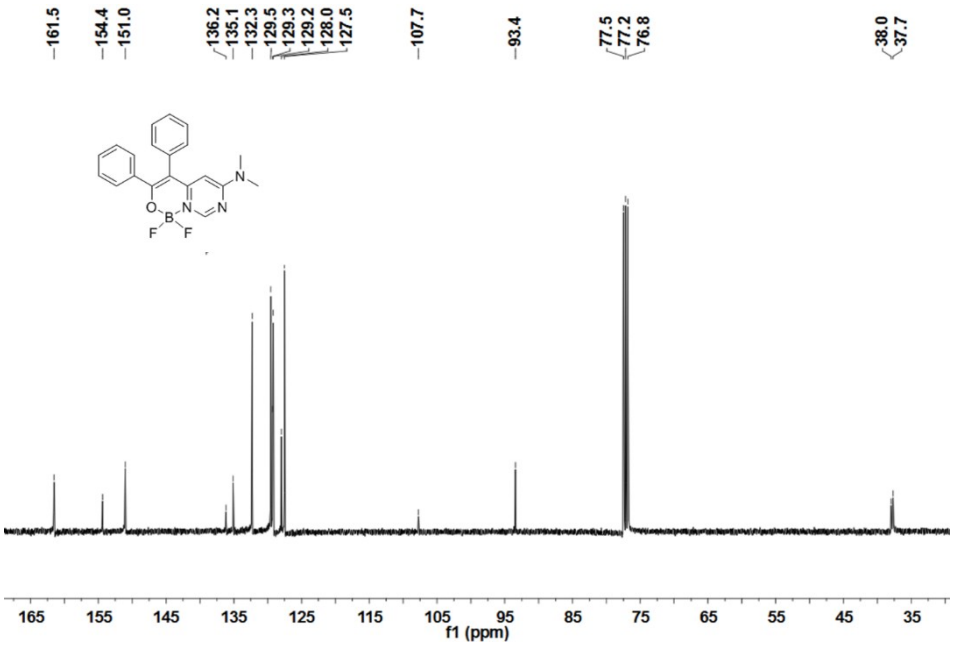


Figure S9. ^{13}C NMR of **PB-3** in $CDCl_3$.

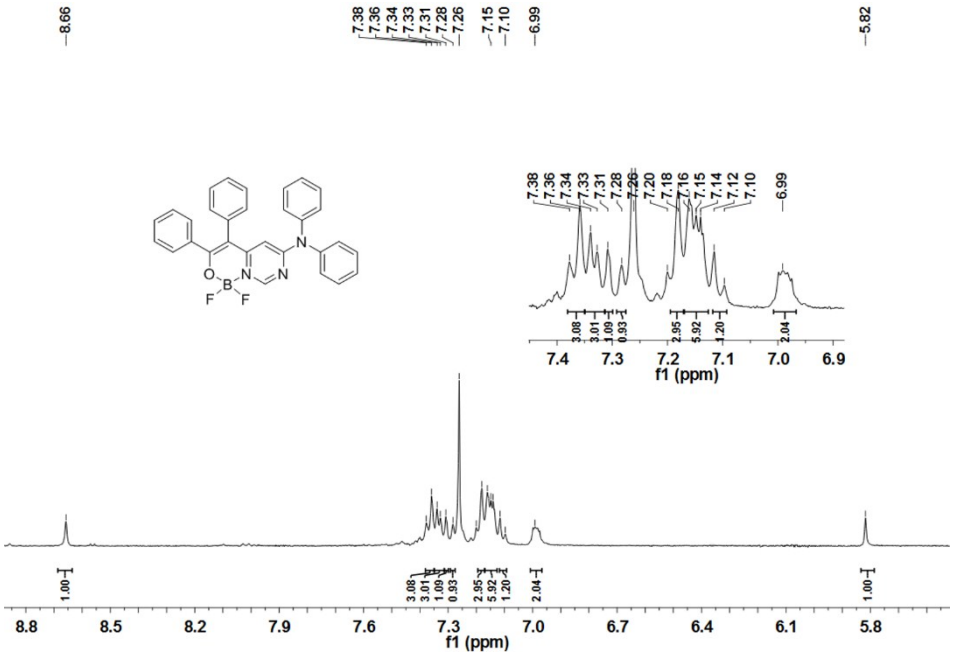


Figure S10. ^{1}H NMR of **PB-4** in $CDCl_3$.

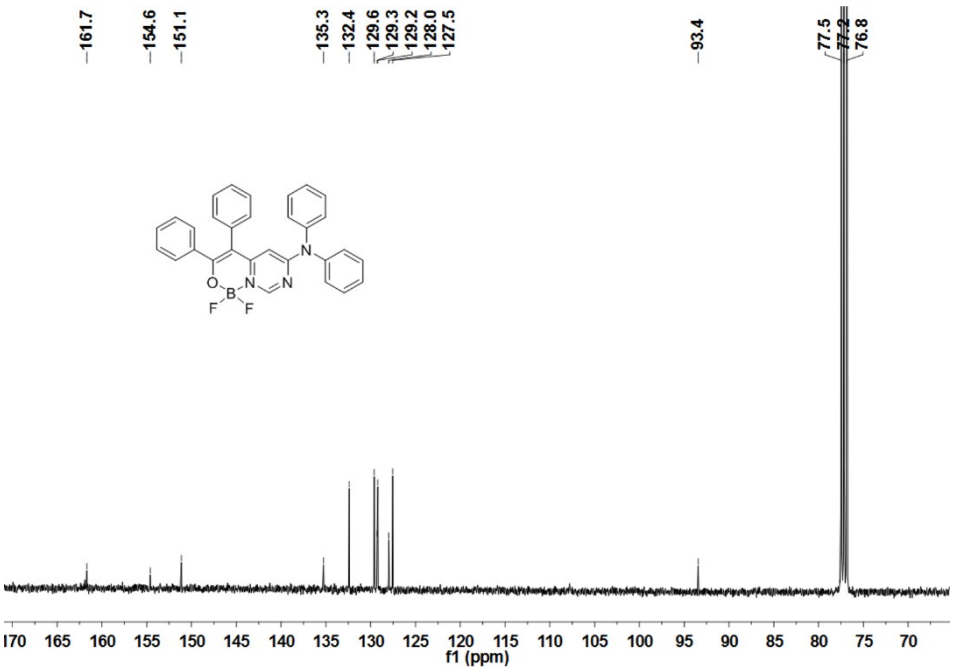
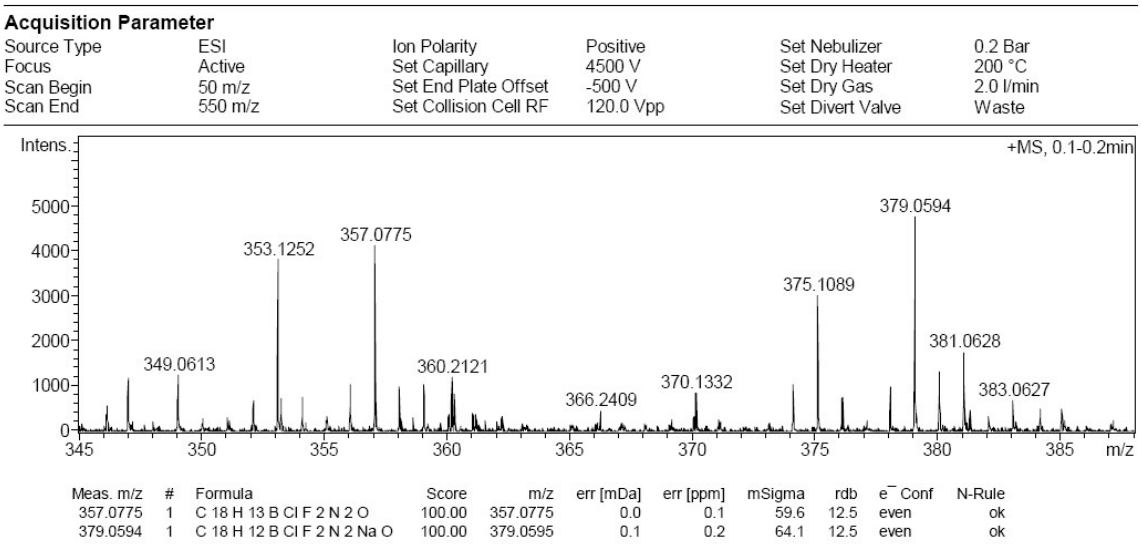
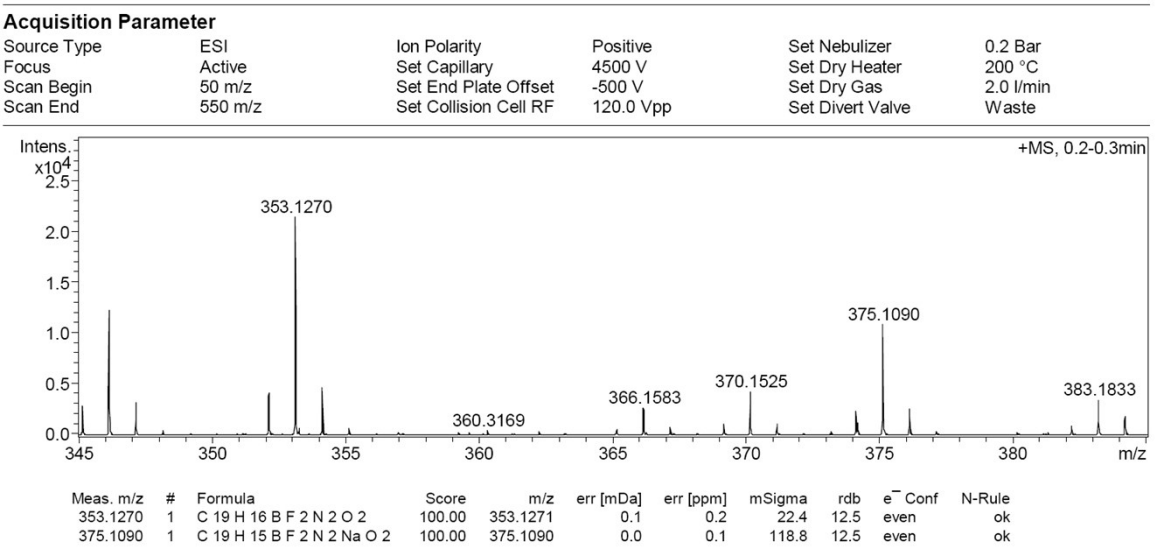


Figure S11. ^{13}C NMR of **PB-4** in $CDCl_3$.



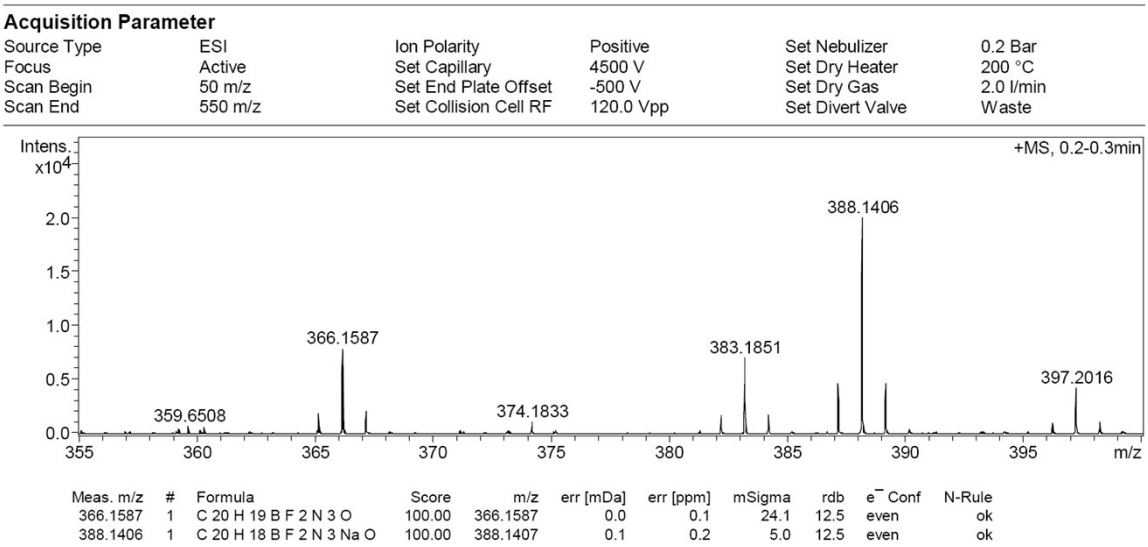
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
357.0775	1	C 18 H 13 B Cl F 2 N 2 O	100.00	357.0775	0.0	0.1	59.6	12.5	even	ok
379.0594	1	C 18 H 12 B Cl F 2 N 2 Na O	100.00	379.0595	0.1	0.2	64.1	12.5	even	ok

Figure S12. HRMS spectrum of **PB-1**.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
353.1270	1	C 19 H 16 B F 2 N 2 O 2	100.00	353.1271	0.1	0.2	22.4	12.5	even	ok
375.1090	1	C 19 H 15 B F 2 N 2 Na O 2	100.00	375.1090	0.0	0.1	118.8	12.5	even	ok

Figure S13. HRMS spectrum of **PB-2**.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
366.1587	1	C 20 H 19 B F 2 N 3 O	100.00	366.1587	0.0	0.1	24.1	12.5	even	ok
388.1406	1	C 20 H 18 B F 2 N 3 Na O	100.00	388.1407	0.1	0.2	5.0	12.5	even	ok

Figure S14. HRMS spectrum of **PB-3.**

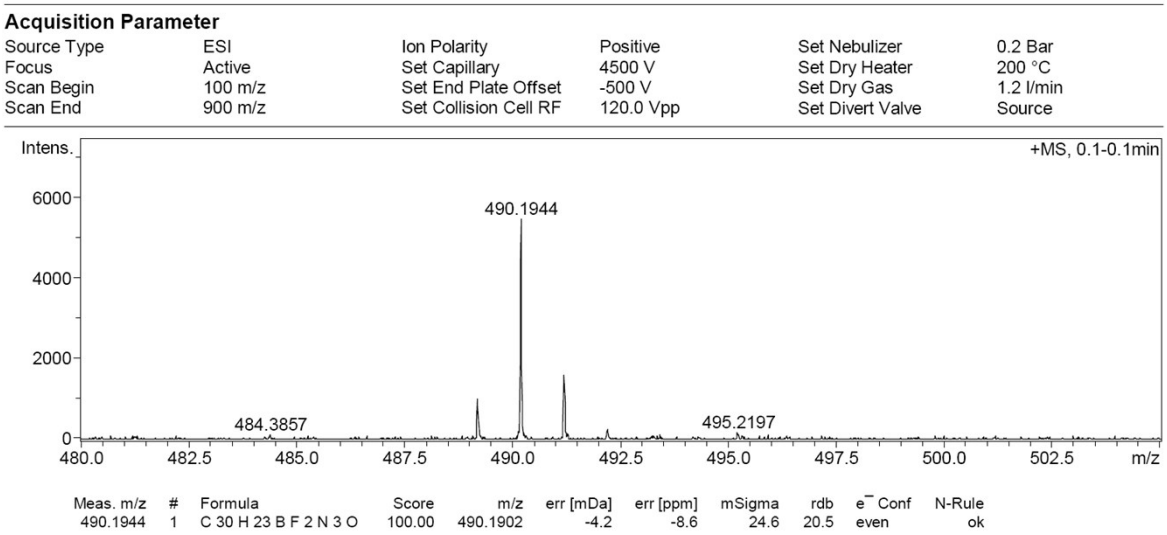


Figure S15. HRMS spectrum of **PB-4.**

Z-matrix and total energy of **PB-1**.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

Cl	-4.88273	1.54284	-0.25072
C	2.47118	-0.75318	-0.00863
O	0.63117	-2.18568	-0.00012
C	-2.31692	0.79208	-0.09431
H	-2.09852	1.69417	-0.14871
C	0.08494	0.11321	0.02058
C	-3.61436	0.40028	-0.1116
C	-1.31397	-0.17269	0.00535
N	-4.00604	-0.87712	-0.0345
C	4.50142	0.3024	0.70502
H	4.9333	0.96229	1.1974
N	-1.72767	-1.47949	0.07423
F	-0.85183	-3.24892	1.40741
C	3.23266	-1.65623	-0.73858
H	2.80811	-2.32726	-1.22405
F	-1.01438	-3.5732	-0.80217
C	4.60192	-1.57351	-0.75238
H	5.09895	-2.18148	-1.25116
B	-0.69496	-2.68341	0.16791
C	1.05725	2.10019	-1.14115
H	1.15066	1.58286	-1.90873
C	5.24044	-0.59239	-0.03107
H	6.16816	-0.53553	-0.04133
C	1.33858	4.18926	-0.03875
H	1.62029	5.07479	-0.05186

C	3.12611	0.22965	0.71812
H	2.63499	0.84123	1.21609
C	0.998	-0.90639	0.01404
C	0.4955	1.54749	-0.00171
C	-3.033	-1.74205	0.05435
H	-3.27711	-2.63836	0.10909
C	0.34689	2.34574	1.10884
H	-0.04796	1.9978	1.87603
C	1.47771	3.40958	-1.14352
H	1.86292	3.76584	-1.91106
C	0.77636	3.65824	1.09804
H	0.68563	4.1832	1.86088

Total Energy, E(TD-HF/TD-KS) = -1562.0490885 Hartree

Z-matrix and total energy of **PB-2**.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	1.69578	-1.40092	0.13679
O	4.44842	1.47097	-0.31226
F	1.04793	-3.46311	-0.85275
O	-0.6387	-2.16313	0.00247
C	-0.59156	1.57591	0.02722
N	3.97187	-0.74824	0.04351
C	1.25741	-0.10335	0.05118
C	-1.03622	-0.89082	0.03418
C	-2.5088	-0.78092	-0.00452
F	0.85406	-3.26146	1.36496
C	3.54889	0.51288	-0.11425
C	-0.15756	0.1478	0.06884
C	2.22431	0.87594	-0.07849
H	1.98123	1.77125	-0.14147
C	-3.23542	-1.68949	-0.76501
H	-2.78745	-2.34355	-1.2509
C	-1.1521	2.11133	-1.11316
H	-1.28235	1.57185	-1.85995
C	-0.41183	2.40347	1.12949
H	-0.03821	2.0591	1.90857
C	3.0153	-1.63671	0.14877
H	3.27926	-2.5238	0.2424
C	-3.21008	0.16561	0.74147
H	-2.74549	0.77856	1.26414
B	0.70395	-2.61726	0.17001
C	-4.61274	-1.6342	-0.80679

H	-5.08721	-2.23416	-1.33646
C	-1.33256	4.24531	-0.06856
H	-1.57772	5.14198	-0.10675
C	-5.28121	-0.69188	-0.0658
H	-6.21024	-0.65531	-0.09029
C	-4.58332	0.19783	0.71241
H	-5.04171	0.82584	1.22111
C	-0.7832	3.73605	1.07771
H	-0.66108	4.2831	1.81991
C	-1.52126	3.43931	-1.15888
H	-1.89969	3.78896	-1.93373
C	5.84247	1.11742	-0.31897
H	6.10501	0.83304	0.55976
H	6.3651	1.87999	-0.57805
H	5.98822	0.40317	-0.9429

Total Energy, E(TD-HF/TD-KS) = -1216.9072323 Hartree

Z-matrix and total energy of **PB-3**.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	-1.29149	-1.71432	-0.07439
O	1.11166	-2.156	0.05562
C	-1.04682	-0.36305	0.04787
C	1.32816	-0.82829	0.02754
C	0.33288	0.07696	0.05855
F	-0.24847	-3.63588	-1.0227
F	-0.34873	-3.50744	1.19196
C	-3.43238	-0.02222	-0.0199
C	2.78881	-0.54219	-0.05756
C	-2.12771	0.48245	0.10664
H	-1.99457	1.39527	0.23127
N	-3.63147	-1.35742	-0.21744
C	0.58318	1.54917	0.10583
C	0.2108	2.36375	-0.95285
H	-0.19495	1.99004	-1.70097
N	-4.51933	0.75284	0.01595
C	-2.56686	-2.1158	-0.20721
H	-2.70739	-3.0294	-0.30273
C	-5.85694	0.21651	-0.17969
H	-5.80059	-0.61956	-0.6489
H	-6.37782	0.83753	-0.6938
H	-6.2734	0.07709	0.67371
C	1.17522	2.13451	1.20054
H	1.43238	1.60503	1.92141

C	3.67157	-1.33758	0.65889
H	3.34019	-2.00276	1.21804
C	0.43631	3.72072	-0.90708
H	0.1926	4.25401	-1.62876
C	5.02982	-1.15377	0.55149
H	5.61196	-1.68366	1.04528
C	3.30496	0.43914	-0.88743
H	2.72651	0.98599	-1.3678
C	4.66311	0.61376	-1.0114
H	4.9985	1.2682	-1.58113
B	-0.17158	-2.78149	0.04322
C	-4.39583	2.17548	0.27469
H	-3.88868	2.31094	1.07879
H	-5.26956	2.55878	0.37871
H	-3.94659	2.59716	-0.46166
C	1.01559	4.28786	0.19365
H	1.15208	5.207	0.22673
C	5.52621	-0.18204	-0.29075
H	6.4451	-0.06208	-0.37201
C	1.39235	3.50194	1.24489
H	1.79508	3.88418	1.9904

Total Energy, E(TD-HF/TD-KS) = -1236.282314 Hartree

Z-matrix and total energy of **PB-4**.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

N	-3.0398	-0.13697	0.10264
N	-1.90055	-2.14772	-0.0159
N	0.45815	-2.18398	-0.0169
C	-1.84942	-0.79538	-0.00483
O	2.89245	-2.26688	0.15976
C	1.82705	-0.19044	-0.14121
C	-4.34899	-0.7357	-0.05187
C	-2.98544	1.28719	0.33143
C	0.52426	-0.82195	-0.08753
C	-0.64564	-0.1299	-0.08283
H	-0.63203	0.79914	-0.13405
C	1.83556	1.29503	-0.30819
C	-4.5973	-1.68296	-1.02313
H	-3.90784	-1.99498	-1.56449
C	-3.20216	2.14591	-0.71492
H	-3.42599	1.81521	-1.55448
F	1.776	-3.9302	-0.82181

C	2.94254	-0.93782	0.00149
C	-6.64646	-0.73525	0.54614
H	-7.34002	-0.40427	1.0732
C	-5.36851	-0.27535	0.72509
H	-5.19454	0.35674	1.38449
C	-2.57075	3.12665	1.757
H	-2.36173	3.46321	2.59822
C	-6.9051	-1.6854	-0.41536
H	-7.76954	-2.00163	-0.54463
C	6.58504	-0.73003	0.82894
H	7.19366	-1.18127	1.36738
C	-0.74049	-2.74895	-0.00233
H	-0.7569	-3.67772	0.01752
C	2.04289	3.49021	0.62082
H	2.2233	4.03645	1.35125
C	4.35262	-0.4487	0.01183
C	2.10346	2.1277	0.75759
H	2.32559	1.75964	1.58251
C	-5.87467	-2.16002	-1.17928
H	-6.04418	-2.81693	-1.81542
C	1.55112	1.86552	-1.52214
H	1.39802	1.32314	-2.26125
C	4.77919	0.61041	-0.76173
H	4.17244	1.06655	-1.29909
C	-2.75722	3.9774	0.71078
H	-2.65745	4.89433	0.83341
C	-2.69226	1.77879	1.56891
H	-2.57569	1.19919	2.2846
B	1.73258	-3.03091	0.14989
C	5.27502	-1.11849	0.80893
H	4.99719	-1.83632	1.33266
C	-3.08788	3.49104	-0.51288
H	-3.23544	4.07644	-1.21862
F	1.64104	-3.69744	1.33871
C	1.48627	3.22359	-1.65443
H	1.28024	3.59728	-2.48087
C	7.00033	0.32008	0.06063
H	7.89314	0.57924	0.07893
C	6.10898	0.99337	-0.73698
H	6.39874	1.70641	-1.26107
C	1.72042	4.04518	-0.57587
H	1.66386	4.96879	-0.66308

Total Energy, E(TD-HF/TD-KS) = -1616.3977003 Hartree