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SUPPORTING INFORMATION

Novel Pyrromethene dyes with N-ethyl carbazole at *meso* position: a comprehensive photophysical, lasing, photostability and TD-DFT study†

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Table S1: Mulliken Charges (e.s.u.) on selected atoms of the dyes **1-3** at their respective optimized ground state and excited state geometries, calculated by using B3LYP/6-31G (d) PCM level of theory in n-heptane

Atom no.	Dye 1		Dye 2		Dye 3	
	GS[a]	ES[b]	GS	ES	GS	ES
C-1	+0.087	+0.091	+0.088	+0.080	+0.097	+0.089
C-2	+0.019	+0.012	+0.015	+0.021	+0.007	+0.014
C-3	+0.316	+0.323	+0.317	+0.316	+0.334	+0.315
N-3'	-0.576	-0.571	-0.579	-0.582	-0.581	-0.583
B-4	+0.693	+0.687	+0.694	+0.694	+0.694	+0.695
C-7'	+0.183	+0.180	+0.215	+0.234	+0.214	+0.234
C-8	+0.115	+0.111	-0.030	-0.037	-0.027	-0.035
C9	-0.015	-0.006	+0.020	+0.016	+0.019	+0.017
C-10	-0.056	-0.059	-0.055	-0.056	-0.123	-0.123
C-11	+0.007	+0.007	+0.005	+0.007	+0.180	+0.181

[a]Mulliken charges of molecules in ground state; [b]Mulliken charges of molecules in excited state

Table S2: Ab initio calculated parameters of PM dyes **2-3** in solvents of different polarities using TD-DFT (B3LYP/6-31G(d)) PCM method

Solvent	Dye 2					Dye 3				
	E_H [a] (eV)	E_L [b] (eV)	E_H-E_L (eV)	μ_0 [c] (Debye)	μ_1 [d] (Debye)	E_H (eV)	E_L (eV)	E_H-E_L (eV)	μ_0 (Debye)	μ_1 (Debye)
DMSO	-5.365	-2.421	2.944	8.445	9.236	-5.4348	-2.4865	2.9483	8.620	9.254
DMF	-5.361	-2.417	2.944	8.426	9.206	-5.4315	-2.4835	2.9480	8.600	9.230
ACN	-5.361	-2.417	2.944	8.422	9.207	-5.4310	-2.4830	2.9480	8.596	9.225
MeOH	-5.359	-2.415	2.944	8.413	9.195	-5.4296	-2.4816	2.9480	8.586	9.214
EtOH	-5.355	-2.412	2.943	8.381	9.153	-5.4225	-2.4735	2.9491	8.551	9.173
Acetone	-5.349	-2.405	2.943	8.352	9.111	-5.4198	-2.4721	2.9477	8.521	9.138
EtOAc	-5.289	-2.349	2.941	7.987	8.661	-5.3638	-2.4177	2.9461	8.128	8.558
$CHCl_3$	-5.270	-2.330	2.940	7.861	8.506	-5.3453	-2.4000	2.9453	7.998	8.414
Dioxane	-5.186	-2.250	2.935	7.293	7.806	-5.2658	-2.3235	2.9423	7.405	7.768
Heptane	-5.167	-2.235	2.932	7.151	7.636	-5.2473	-2.3067	2.9407	7.264	7.608

[a]Energy of highest occupied molecular orbital (HOMO); [b] Energy of lowest unoccupied molecular orbital (LUMO); [c]Dipole moment in ground state (S_0); [d]Dipole moment in excited state (S_1).

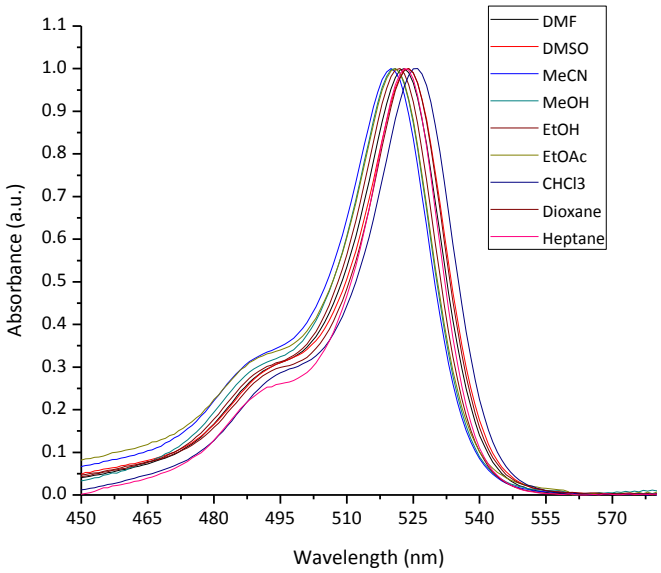


Fig. S1 Normalized absorption spectra of the dye **2** in various solvents

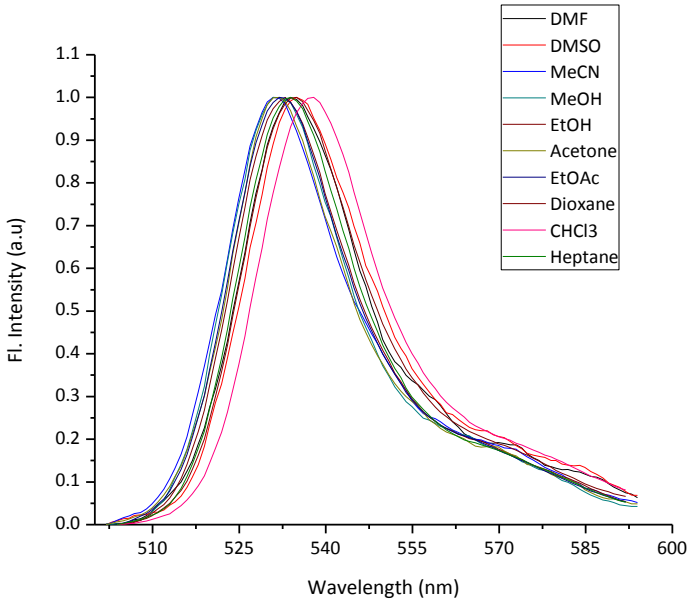


Fig. S2 Normalized emission spectra of the dye **2** in various solvents

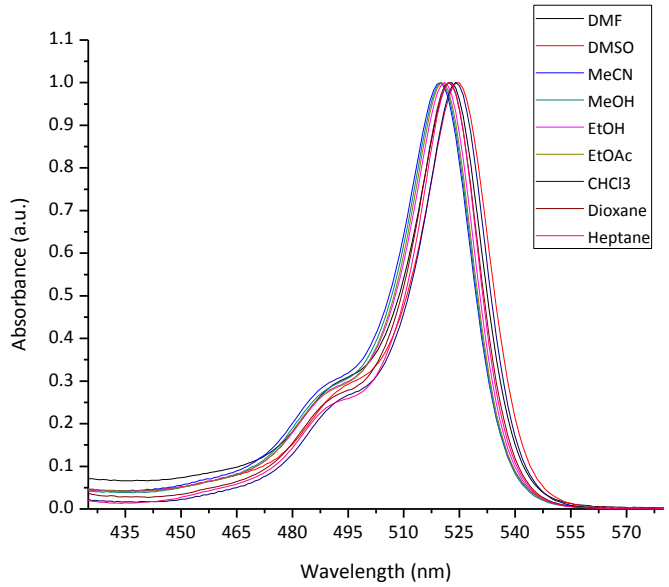


Fig. S3 Normalized absorption spectra of the dye **3** in various solvents

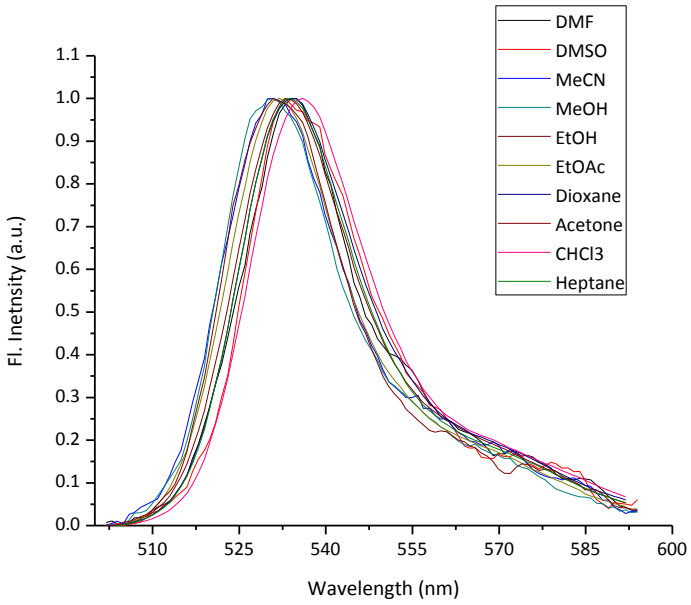


Fig. S4 Normalized emission spectra of the dye **3** in various solvents

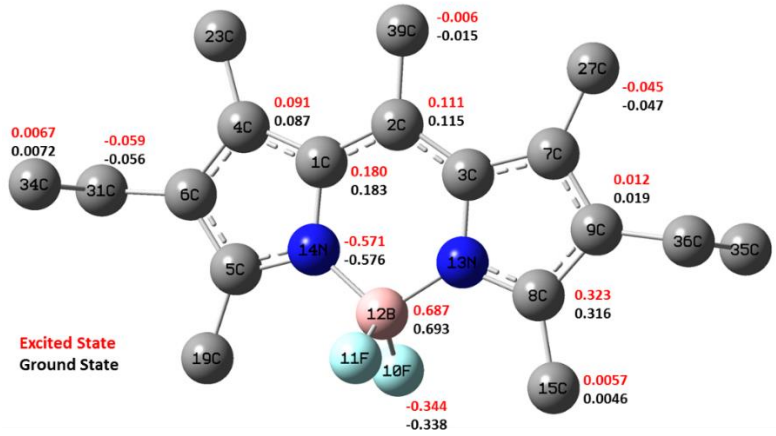


Fig. S5 Optimized structure in ground (S_0) state and Mulliken charges (e.s.u) of the dye **1** in ground state (S_0) (black digits) and first excited state (S_1) (red digits) in solvent n-heptane, calculated by B3LYP/6-31G(d)level of theory (hydrogen atoms are omitted for more clarity).

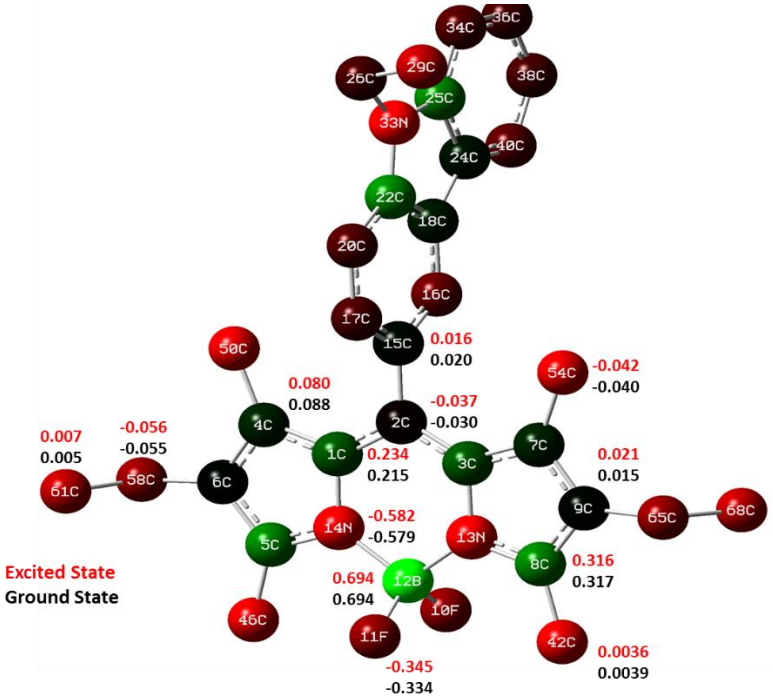


Fig. S6 Optimized structure in ground (S_0) state and Mulliken charges (e.s.u) of the dye **2** in ground state (S_0) (black digits) and first excited state (S_1) (red digits) in solvent n-heptane, calculated by B3LYP/6-31G(d)level of theory (hydrogen atoms are omitted for more clarity).

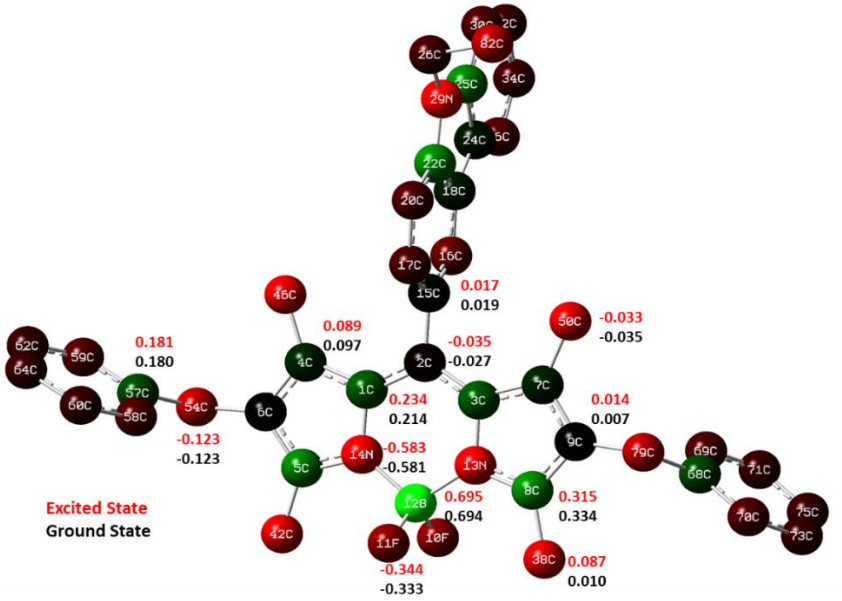


Fig. S7 Optimized structure in ground (S_0) state and Mulliken charges (e.s.u) of the dye **3** in ground state (S_0) (black digits) and first excited state (S_1) (red digits) in solvent n-heptane, calculated by B3LYP/6-31G(d)level of theory (hydrogen atoms are omitted for more clarity).

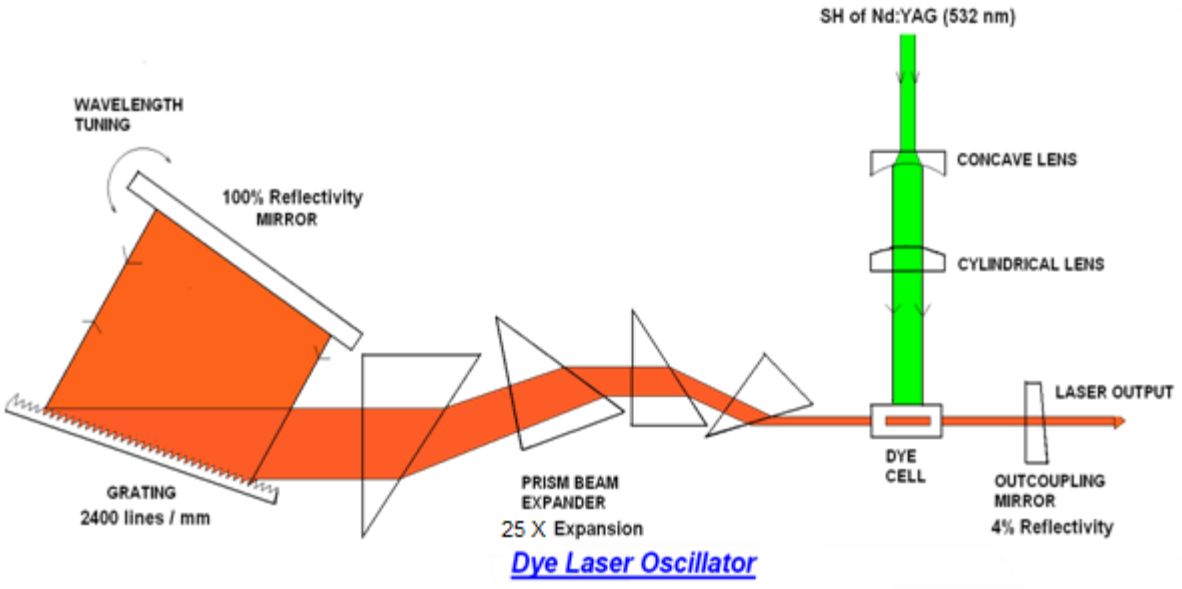
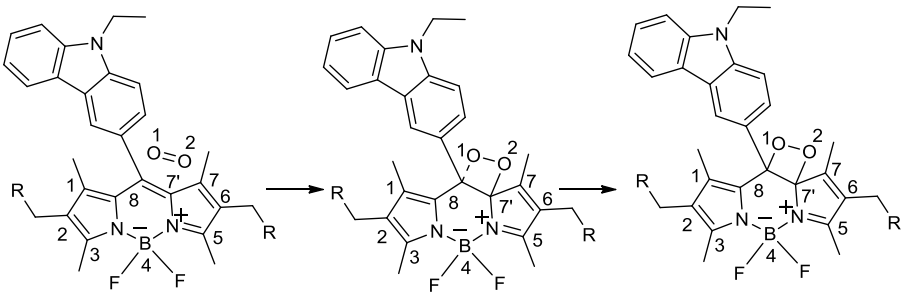


Fig. 8 A schematic of narrow band dye laser set up used for experiments



Dye**2**; R=CH_3
Dye**3**; R=C_5H_5

Fig. S9 Plausible reaction mechanism of the dyes **2** and **3** with $^1O_2$

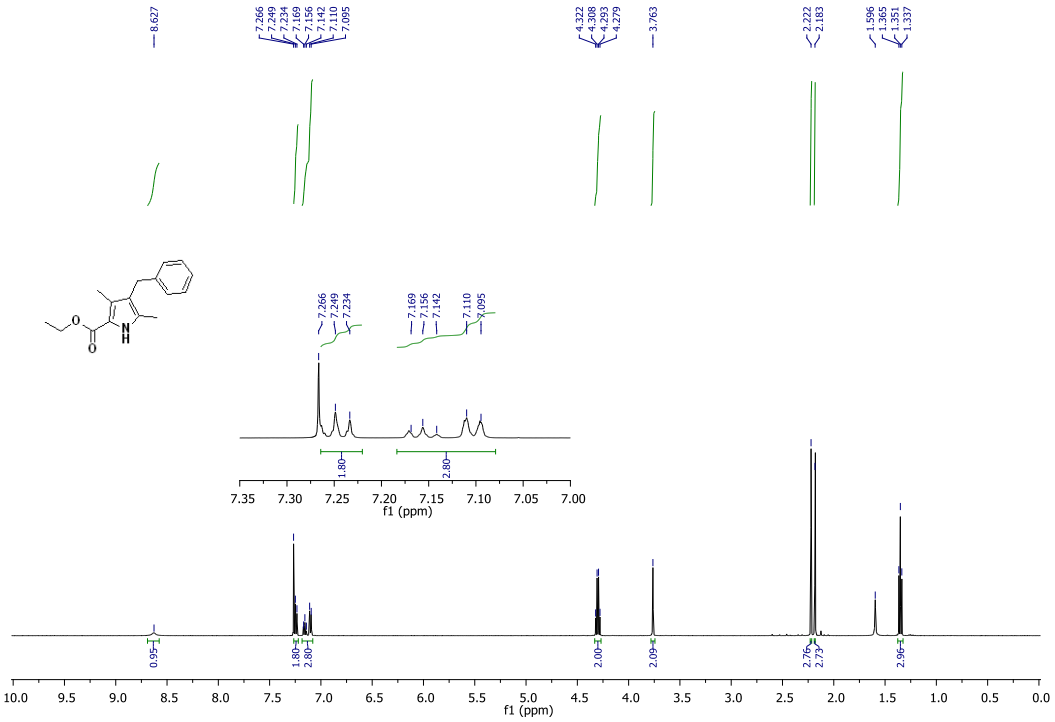


Fig. 10 ^{1}H NMR spectrum of Ethyl 4-benzyl-3, 5-dimethyl-1H-pyrrole-2-carboxylate (**6**)

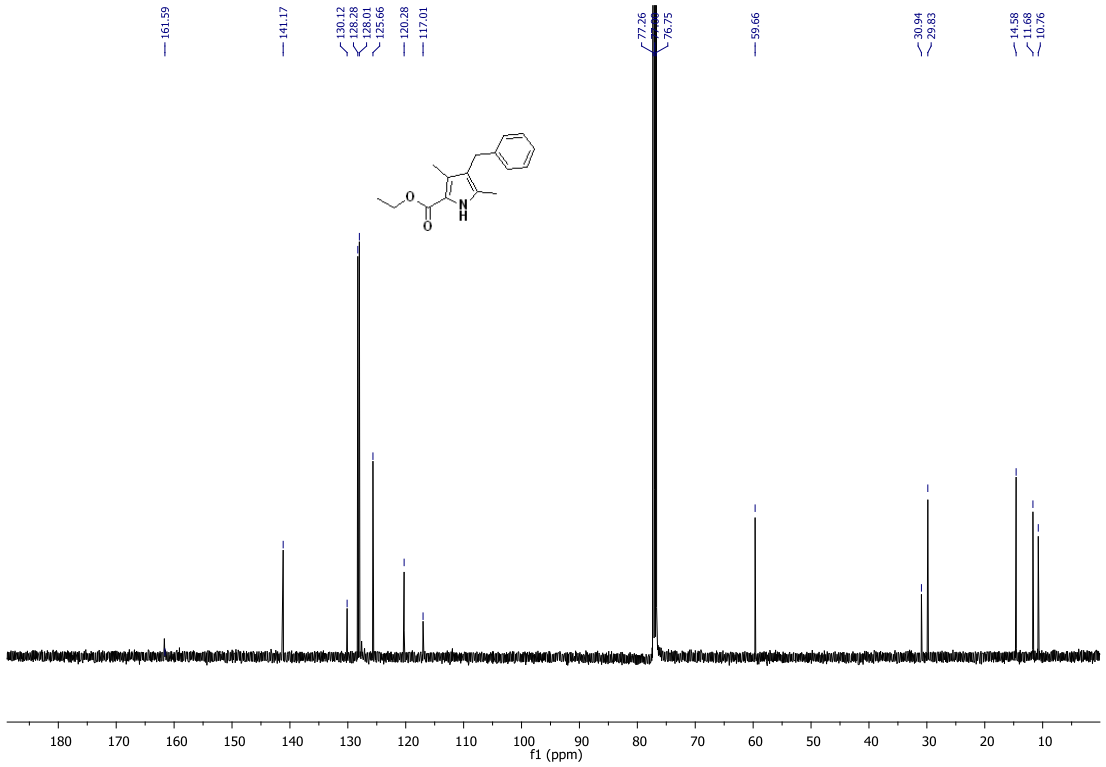


Fig. S11 ^{13}C NMR spectrum of Ethyl 4-benzyl-3, 5-dimethyl-1H-pyrrole-2-carboxylate (**6**)

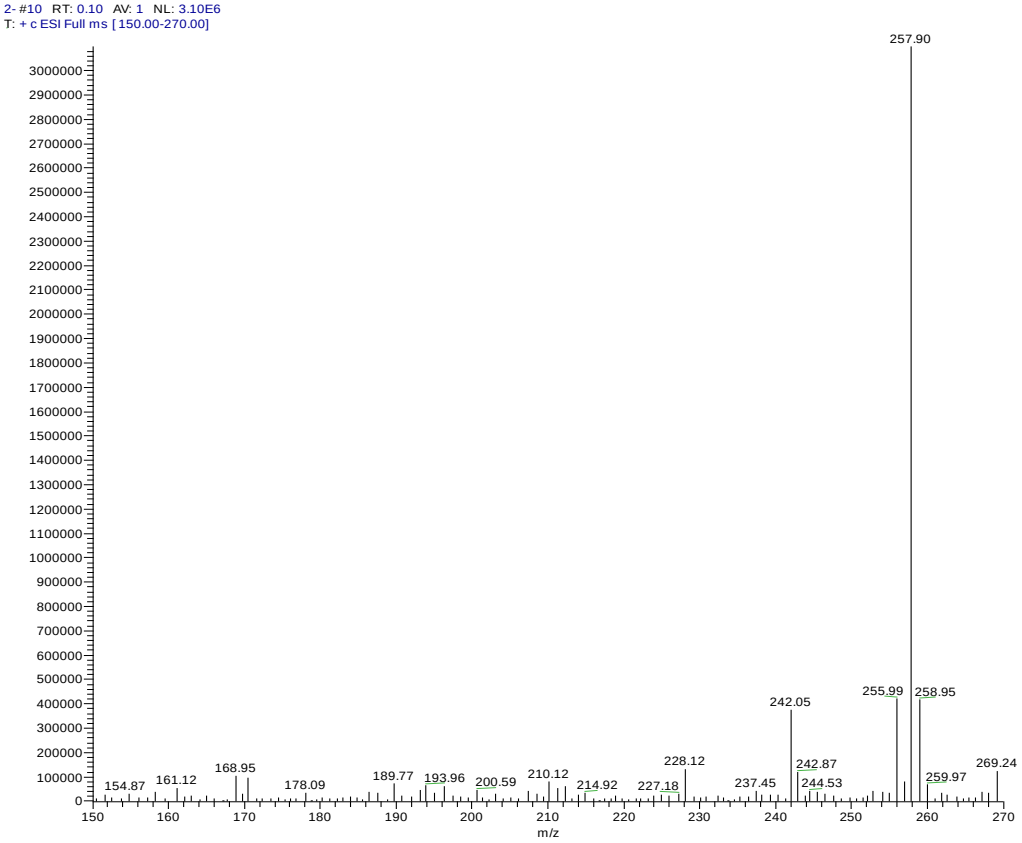


Fig. S12 Mass spectrum of Ethyl 4-benzyl-3, 5-dimethyl-1H-pyrrole-2-carboxylate (**6**)

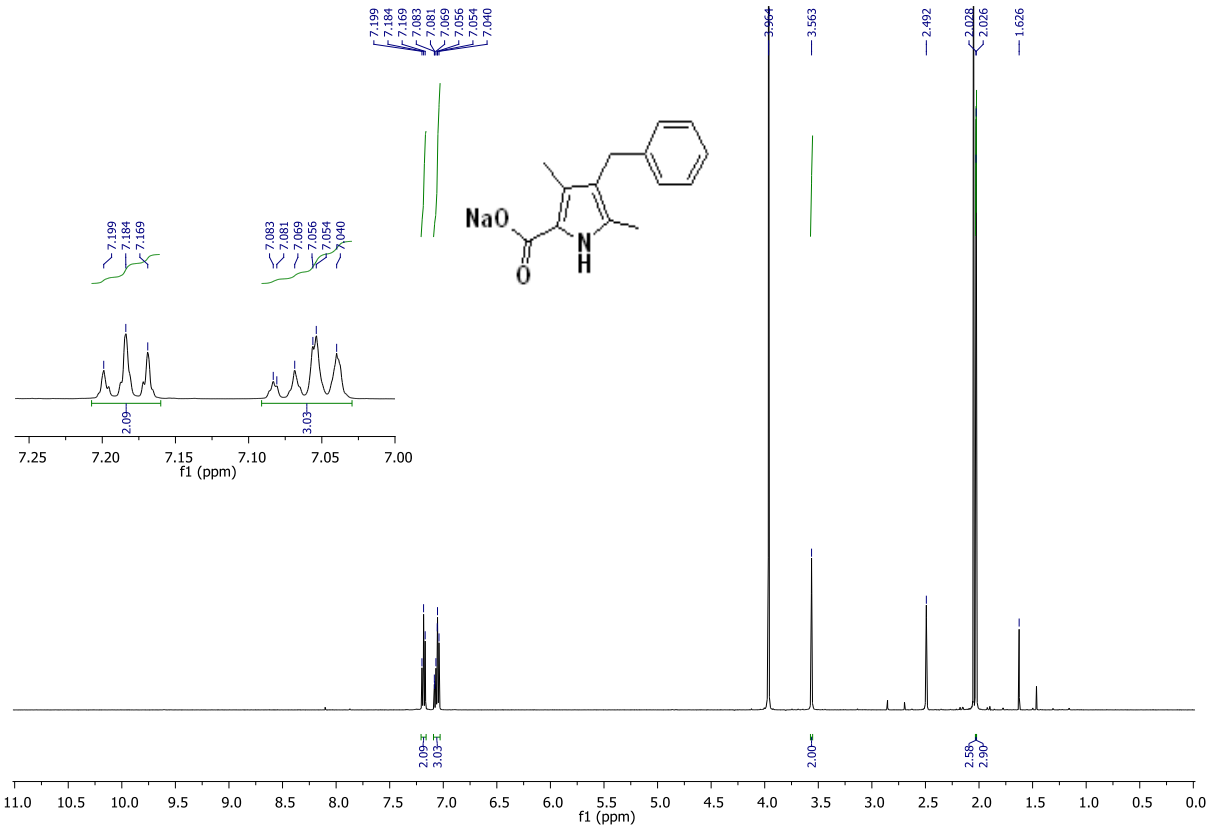


Fig. S13 ^{1}H NMR spectrum of sodium 4-benzyl-3, 5-dimethyl-1H-pyrrole-2-carboxylate (**7**)

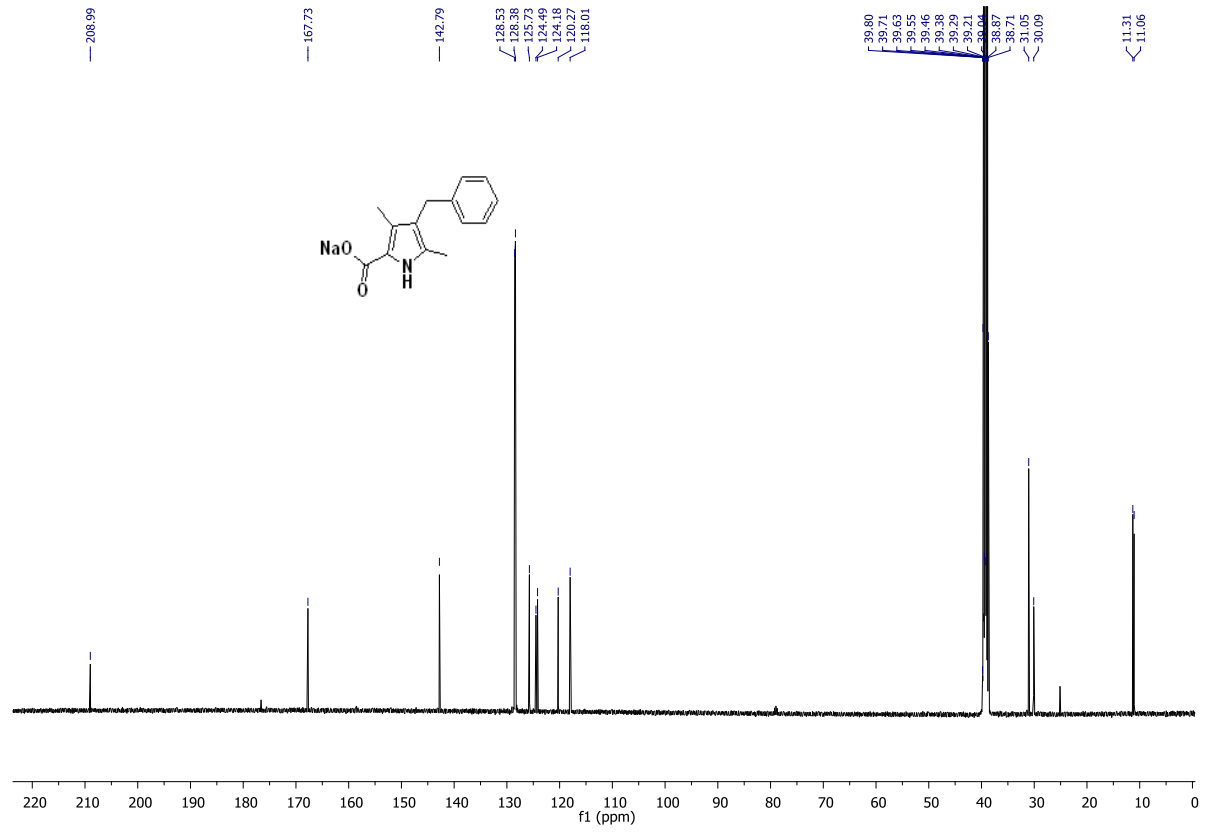


Fig. S14 ^{13}C NMR spectrum of sodium 4-benzyl-3, 5-dimethyl-1H-pyrrole-2-carboxylate (**7**)

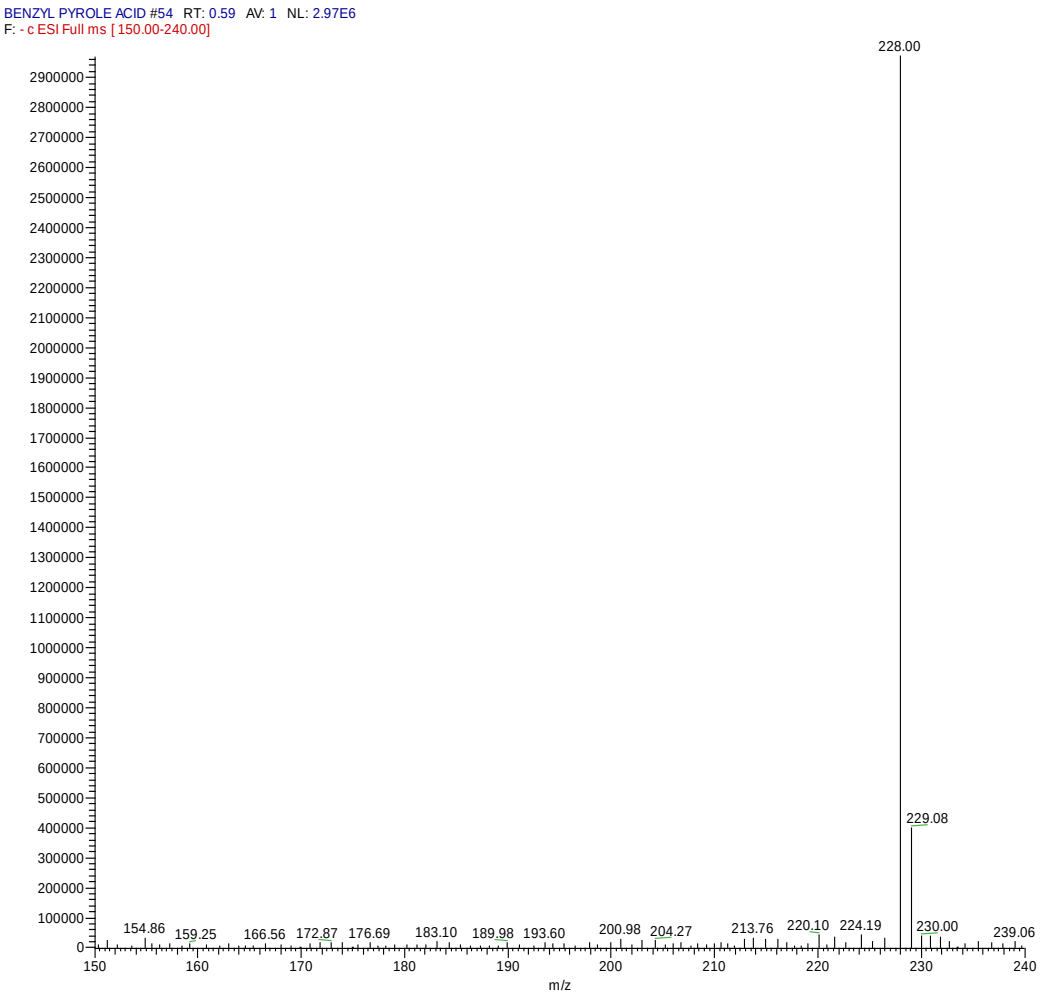


Fig. S15 Mass spectrum of sodium 4-benzyl-3, 5-dimethyl-1H-pyrrole-2-carboxylate (**7**)

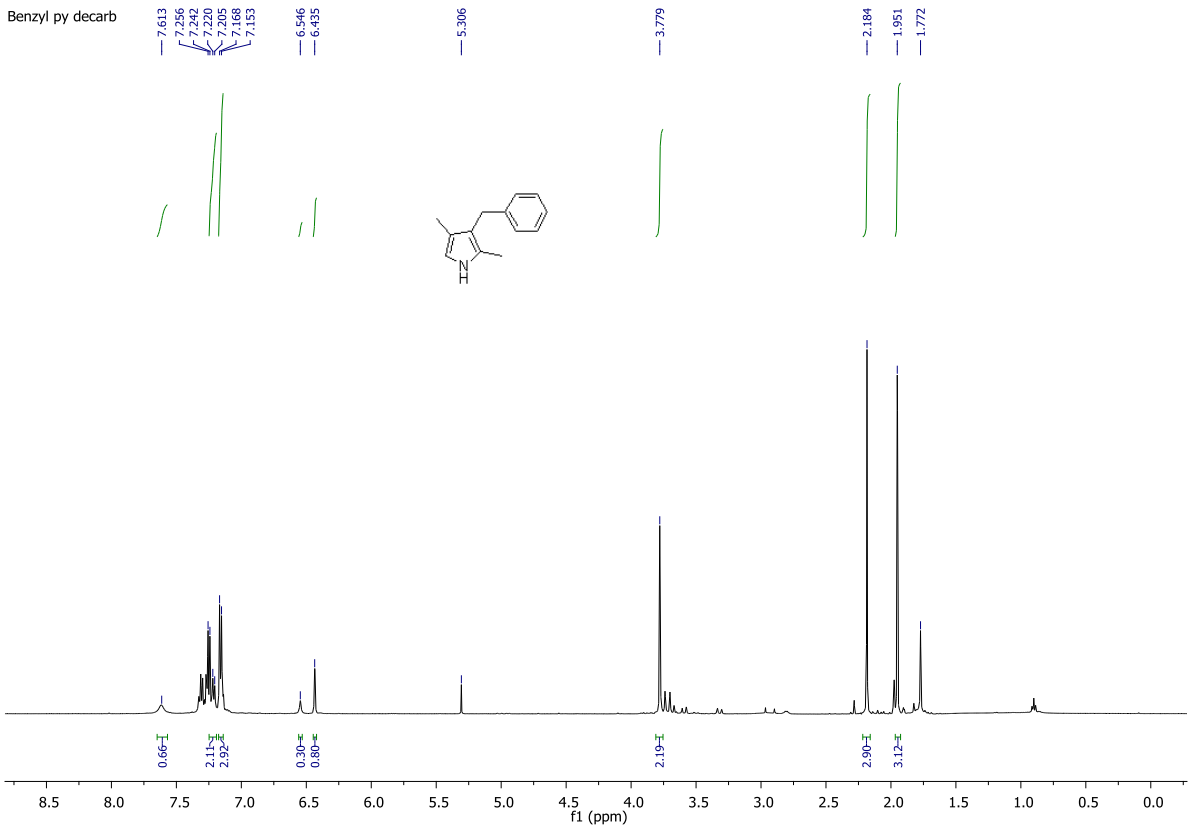


Fig. S16 ^{1}H NMR spectrum of 3-Benzyl-2, 4-dimethyl-1H-pyrrole (**8**)

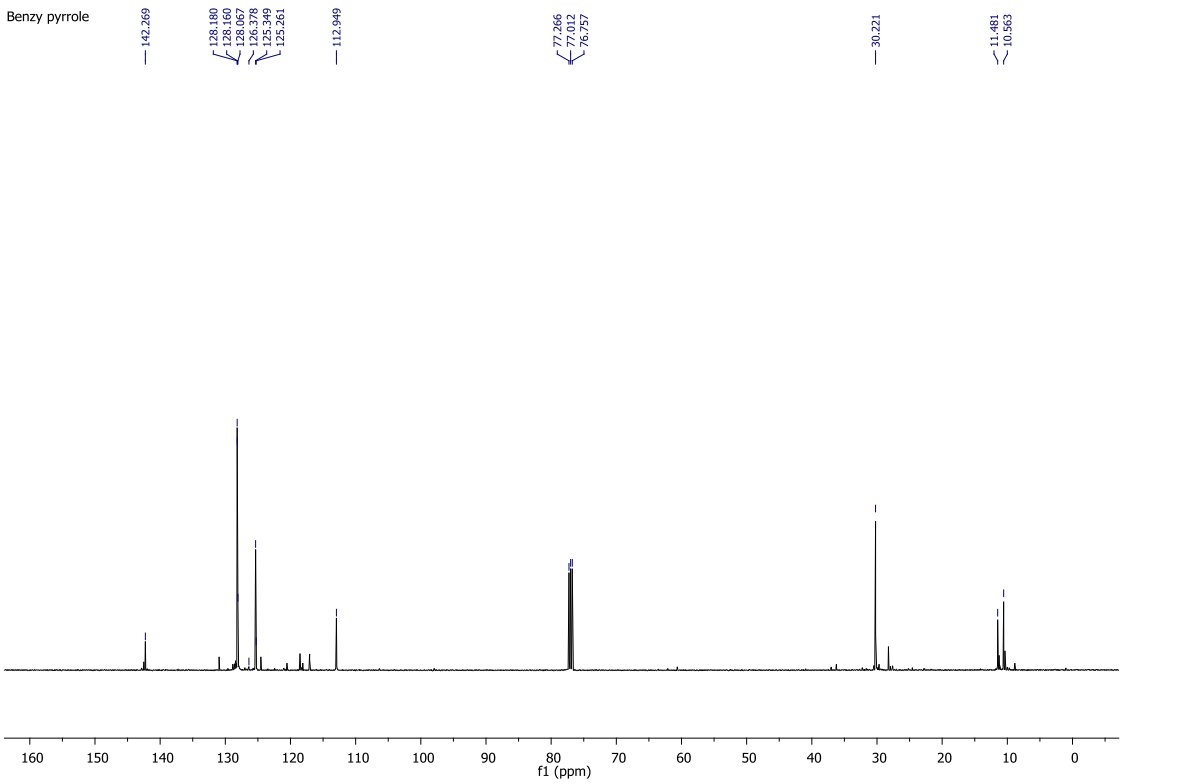


Fig. S17 ^{13}C NMR spectrum of 3-Benzyl-2, 4-dimethyl-1H-pyrrole (**8**)

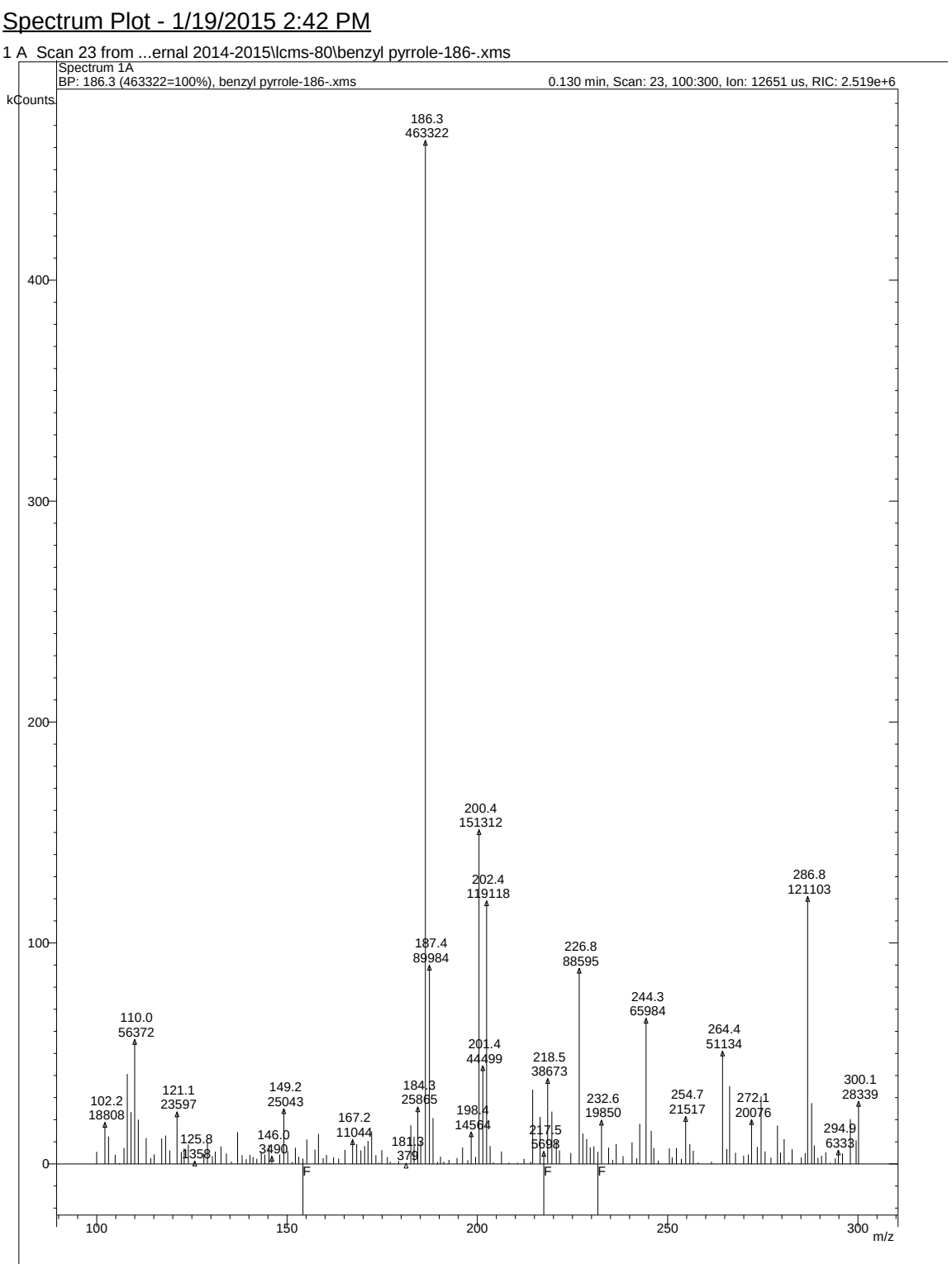


Fig. S18 Mass spectrum of3-Benzyl-2, 4-dimethyl-1H-pyrrole (**8**)

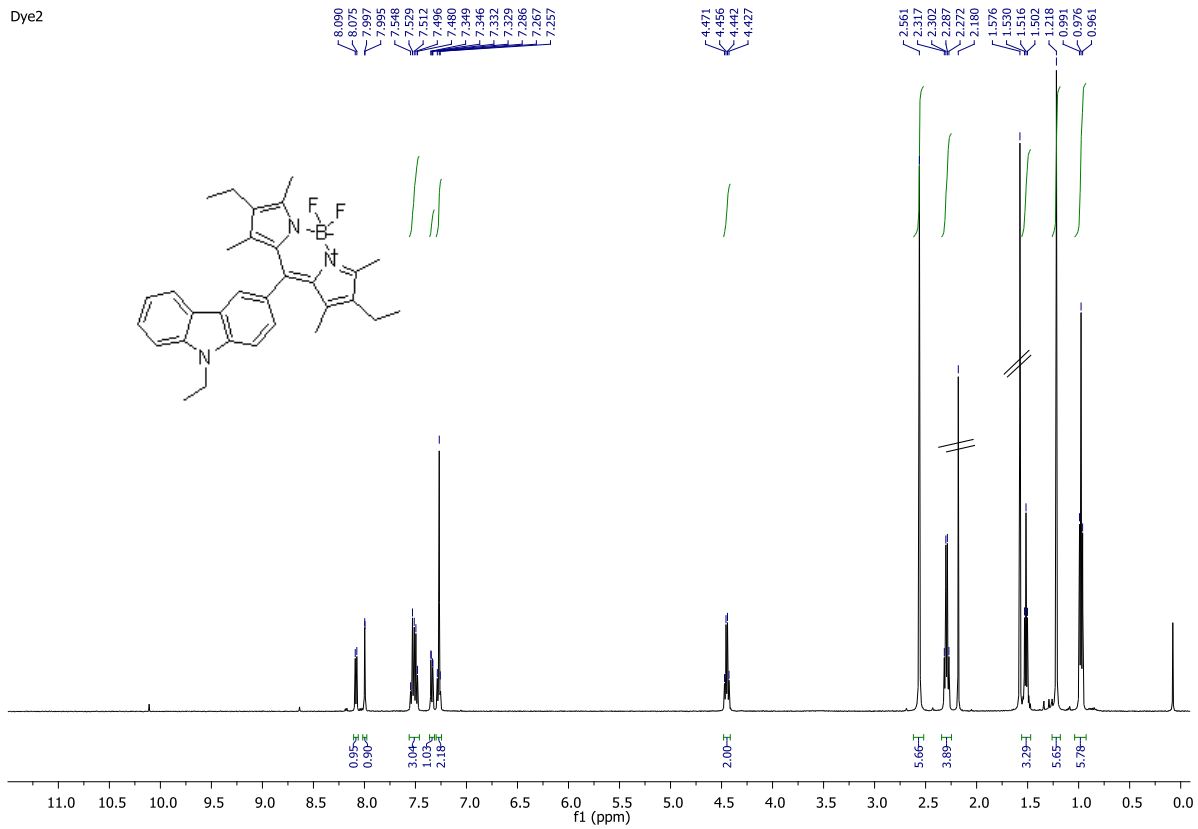


Fig. S19 ^{1}H NMR spectrum of the dye **2.**

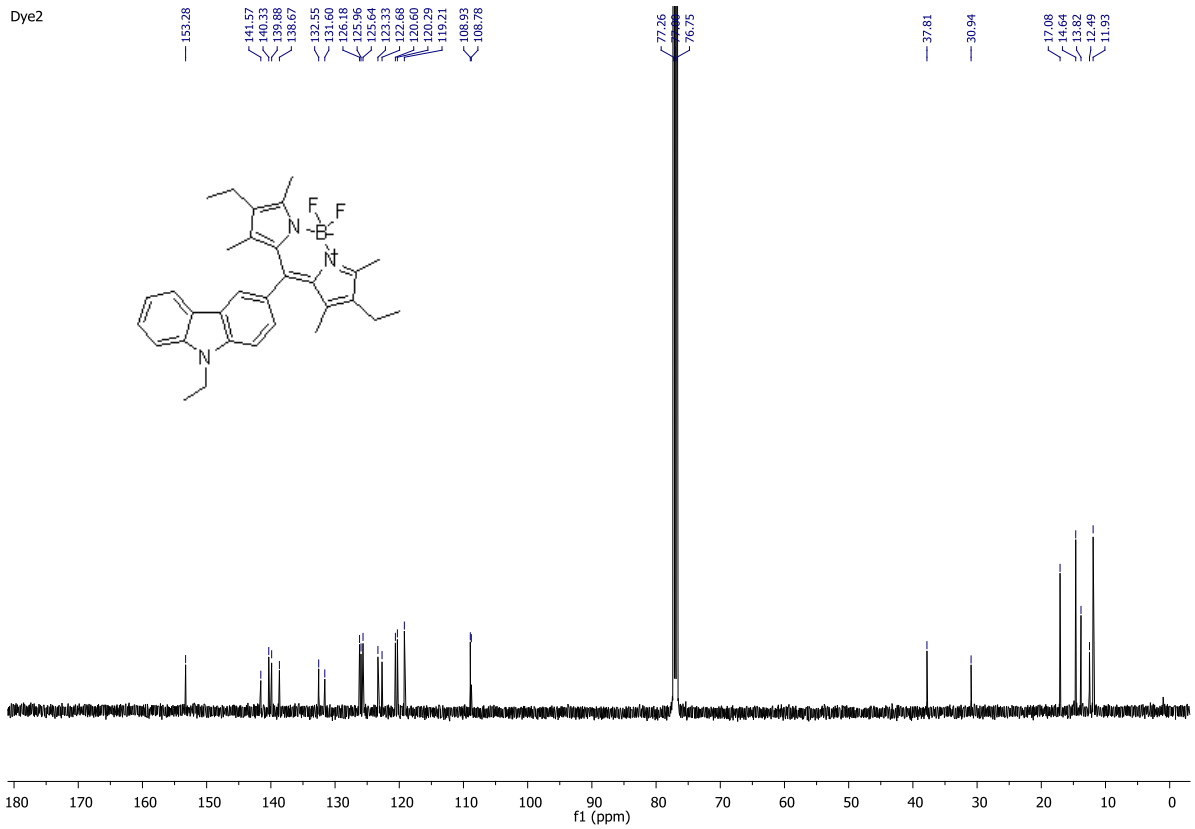


Fig. S20 ^{13}C NMR spectrum of the dye **2**.

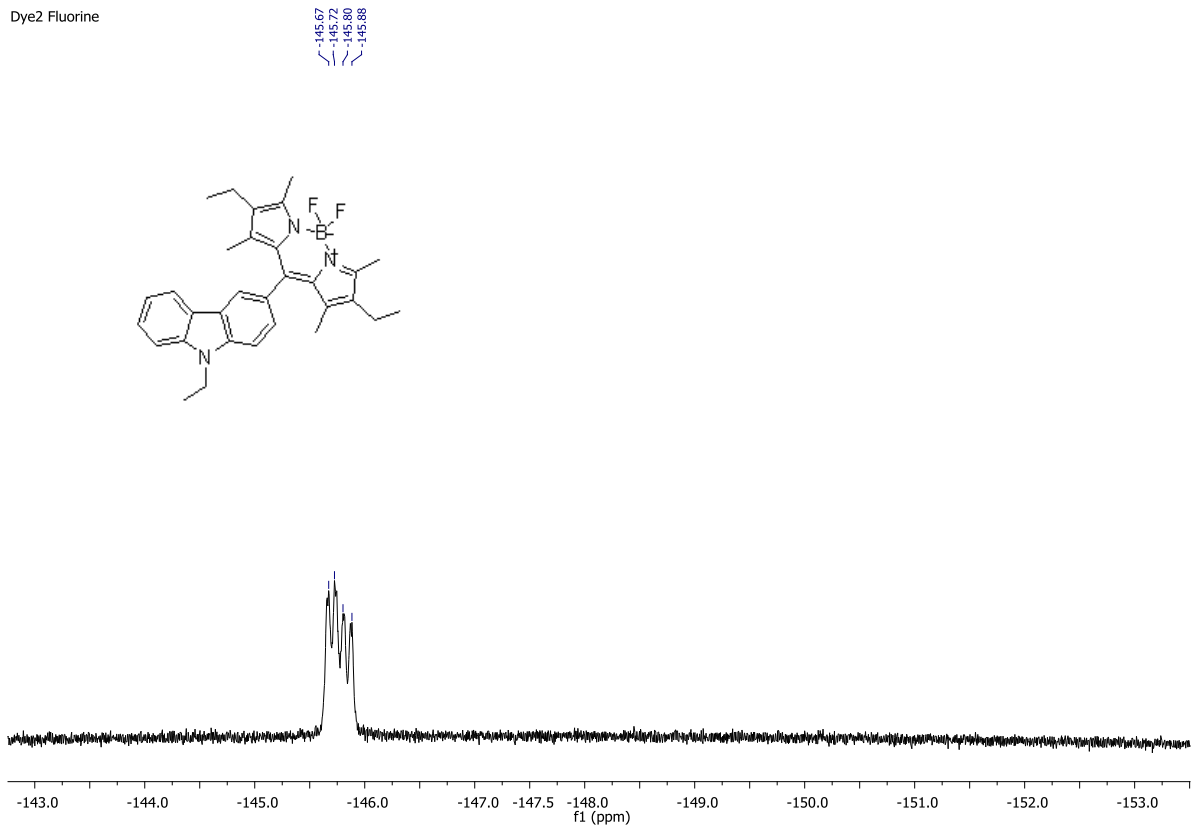
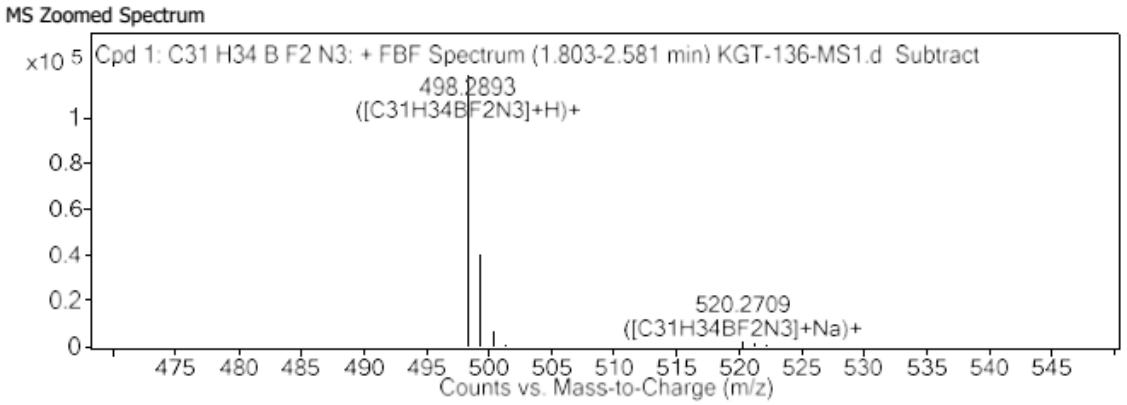


Fig. S21 ^{19}F NMR spectrum of the dye **2**.



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
498.2893	1	118870.19	C31H34BF2N3	(M+H)+
499.2921	1	40134.95	C31H34BF2N3	(M+H)+
500.2952	1	6948.03	C31H34BF2N3	(M+H)+
501.2988	1	771.98	C31H34BF2N3	(M+H)+
520.2709	1	2051.9	C31H34BF2N3	(M+Na)+
521.2742	1	967.78	C31H34BF2N3	(M+Na)+
522.2763	1	537.07	C31H34BF2N3	(M+Na)+

Fig. S22 HRMS spectrum of the dye **2**.

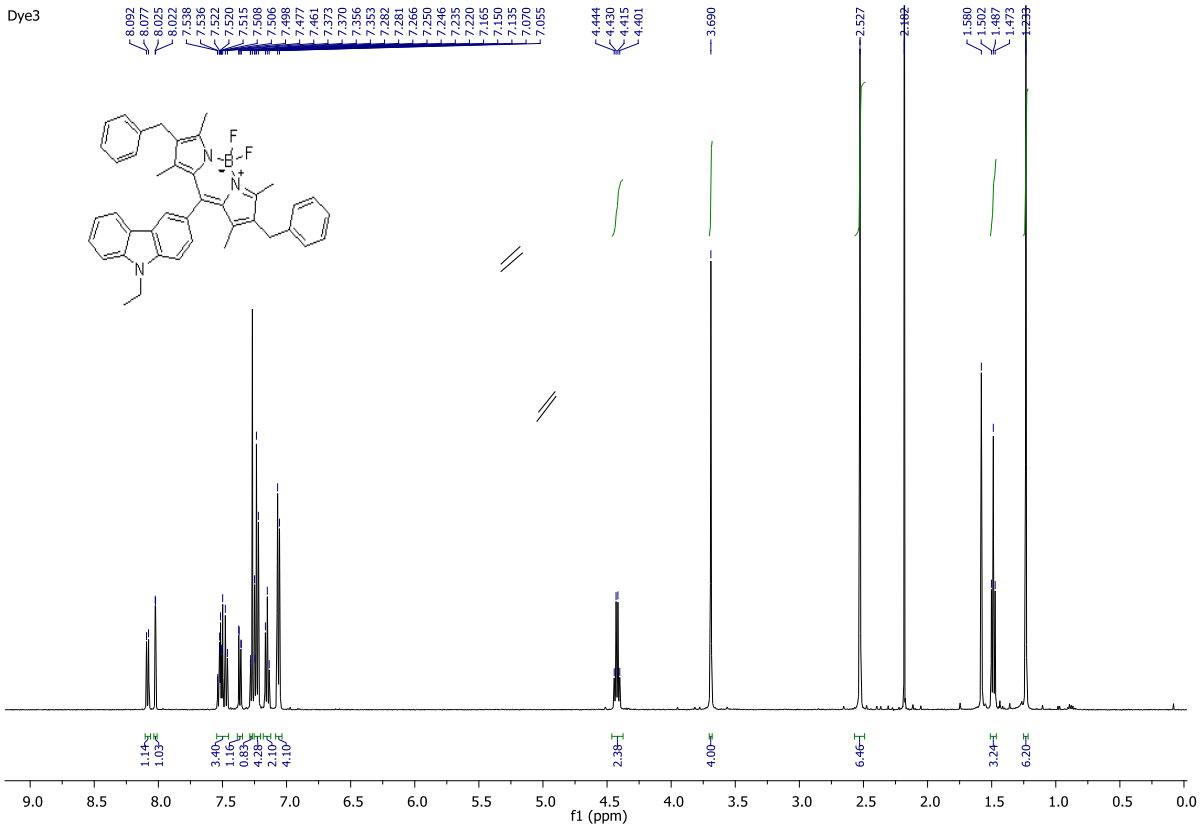


Fig. S23 ^{1}H NMR spectrum of the dye **3**.

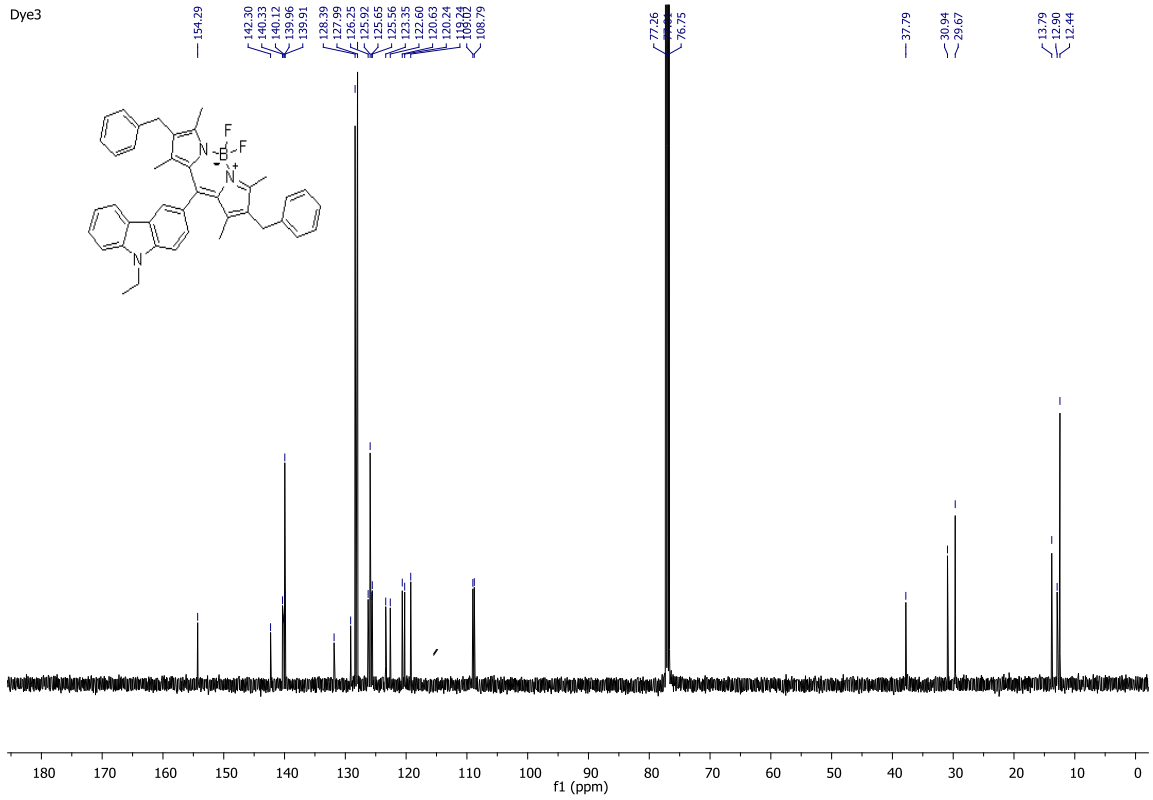


Fig. S24 ^{13}C NMR spectrum of the dye **3**.

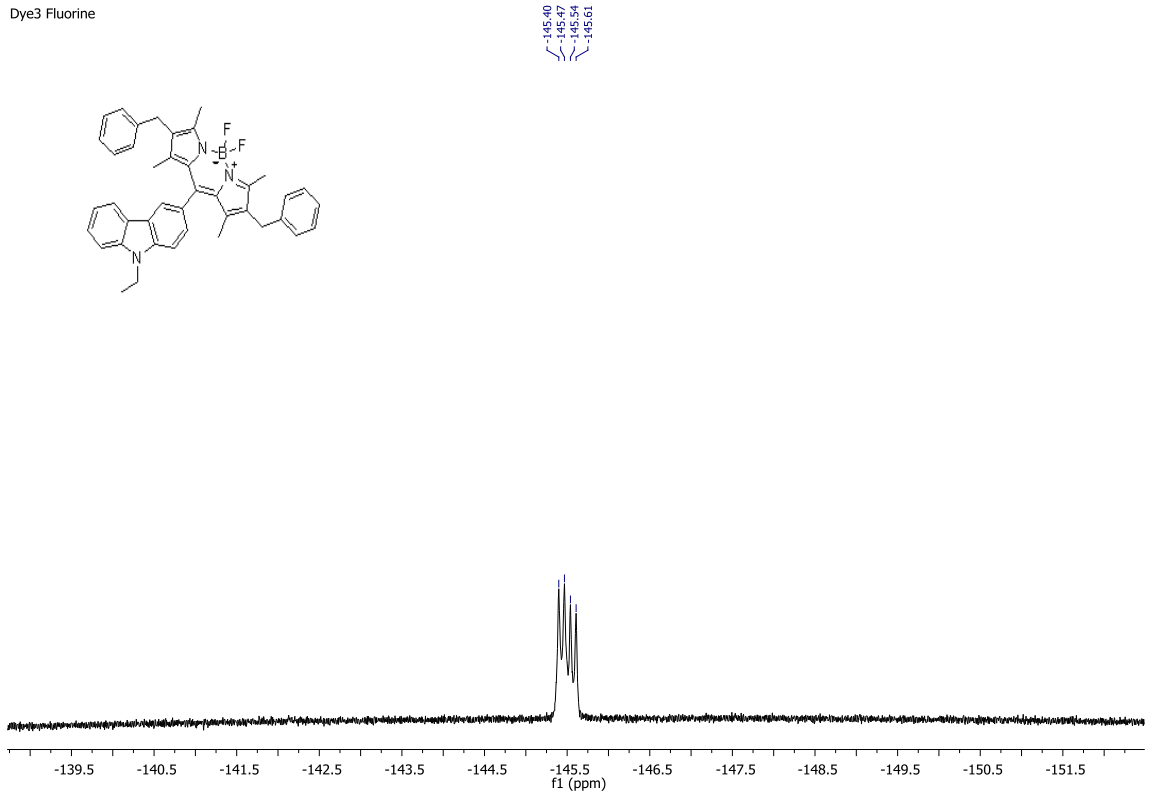
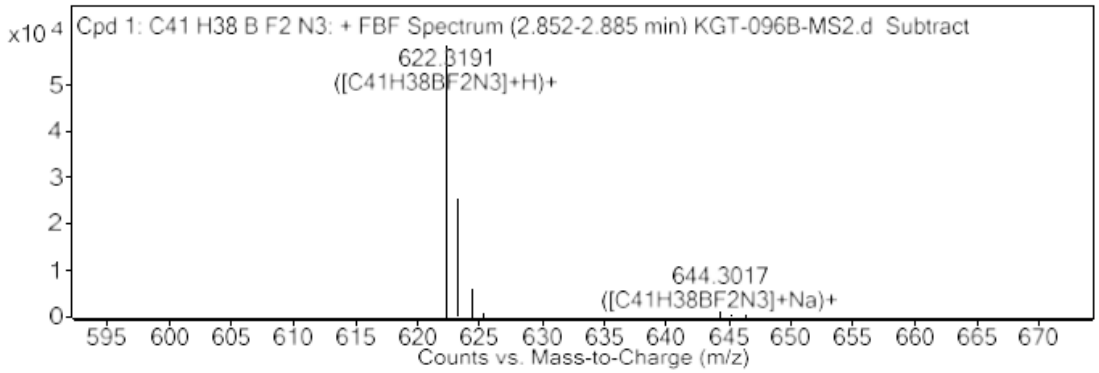


Fig. S25 ^{19}F NMR spectrum of the dye **3**.

MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
622.3191	1	58282.21	C41H38BF2N3	(M+H)+
623.3221	1	25492.14	C41H38BF2N3	(M+H)+
624.3247	1	5864.28	C41H38BF2N3	(M+H)+
625.3301	1	605.49	C41H38BF2N3	(M+H)+
644.3017	1	810.02	C41H38BF2N3	(M+Na)+
645.3052	1	546.92	C41H38BF2N3	(M+Na)+
646.316	1	430.4	C41H38BF2N3	(M+Na)+

Fig. S26 HRMS spectrum of the dye **3**.