Supporting Information

Trans- A_2B – Corrole Bearing 2,3-di(2-pyridyl)quinoxaline(DPQ) / Phenothiazine Moiety's: Synthesis, Characterization, Electrochemistry and Photophysics

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Table S1. Singlet excited state properties of F10C-PTZ and F10C-DPQ dyads by B3LYP method in dichloromethane solvent.

Sample	[a]λ_{max}	[b]f	[c]E eV	% of Molecular Orbital Contribution
F10C-PTZ	306	0.073	4.04	H-2 →L+2 (26%), H-1→L+2 (48%), H-11→LUMO (6%), H-1→L+3 (3%), HOMO→L+5 (7%)
	390	1.166	3.17	H-2→L+1 (61%), H-1→L+1 (18%), H-1→LUMO (4%), HOMO→LUMO (8%).
	399	0.84	3.10	H-2→LUMO (18%), H-1→L+1 (43%), HOMO→L+1 (16%)H-1→LUMO (7%).
	449	0.56	2.75	H-2→LUMO (10%), H-2→L+1 (13%), H-1→L+1 (26%), HOMO→L+1 (44%)
	590	0.279	2.10	HOMO→LUMO (86%), H-2→L+1 (3%), H-1→LUMO (3%), H-1→L+1 (6%)
F10C-DPQ	329	0.063	3.76	HOMO →L+4 (86%), H-8→LUMO (4%), H-6 →LUMO (3%)
	352	0.158	3.51	H-5 →L+1 (49%), H-3→L+1 (14%), H-2→L+1 (19%), H-14→L+1 (4%), H-5→L+2 (4%).
	393	1.024	3.15	H-1→L+2 (78%), HOMO→LUMO (11%), H-4→LUMO (2%), H-2→LUMO (3%)
	416	1.421	2.98	H-1→LUMO (29%), HOMO→L+2 (58%), HOMO→L+3 (5%)
	569	0.332	2.17	H-1→L+2 (11%), HOMO→LUMO (78%), H-1→LUMO (5%), HOMO→L+2 (3%)

[a] Theoretical absorbance in nm, [b] Oscillator strength, [c] Excited state energy in eV.

Table S2. $I_{(dyad)} / I_{(ref)}$ values for F10C-PTZ and F10C-DPQ w.r.t. reference compound "tpfc", when excited at 420 nm.

	CH2Cl2	PhMe	MeCN	DMF
F10C-PTZ	0.29	0.57	0.40	0.38
F10C-DPQ	0.39	0.55	0.0060	0.0034

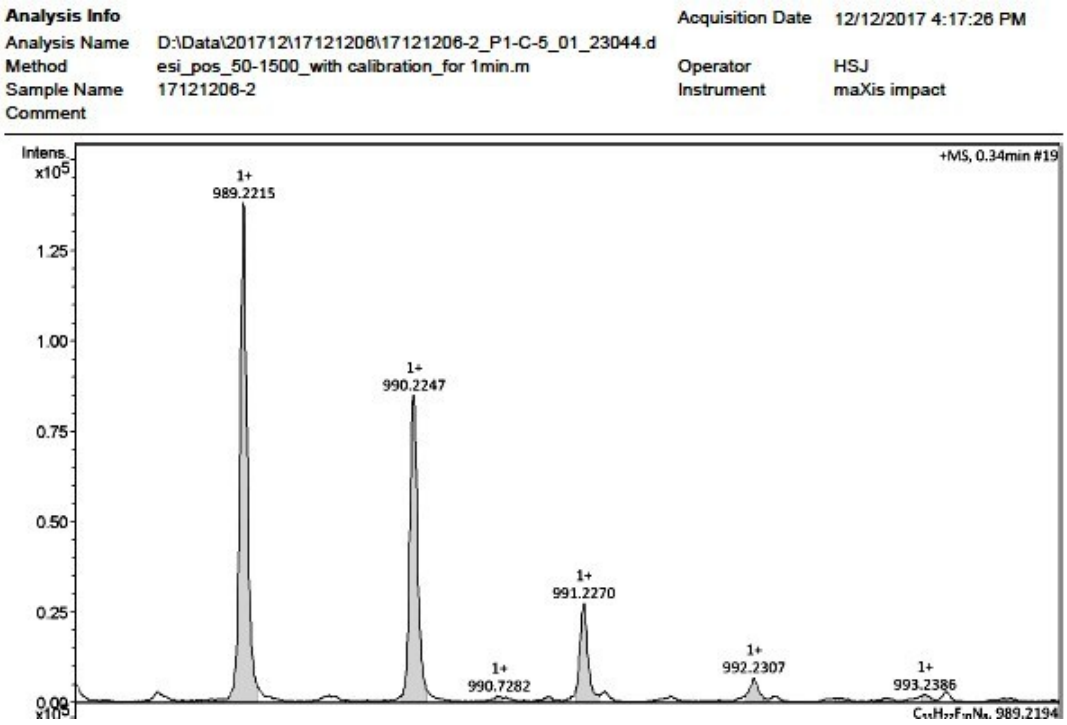

Fig. S1: HRMS Spectrum of F10C-DPQ dyad.

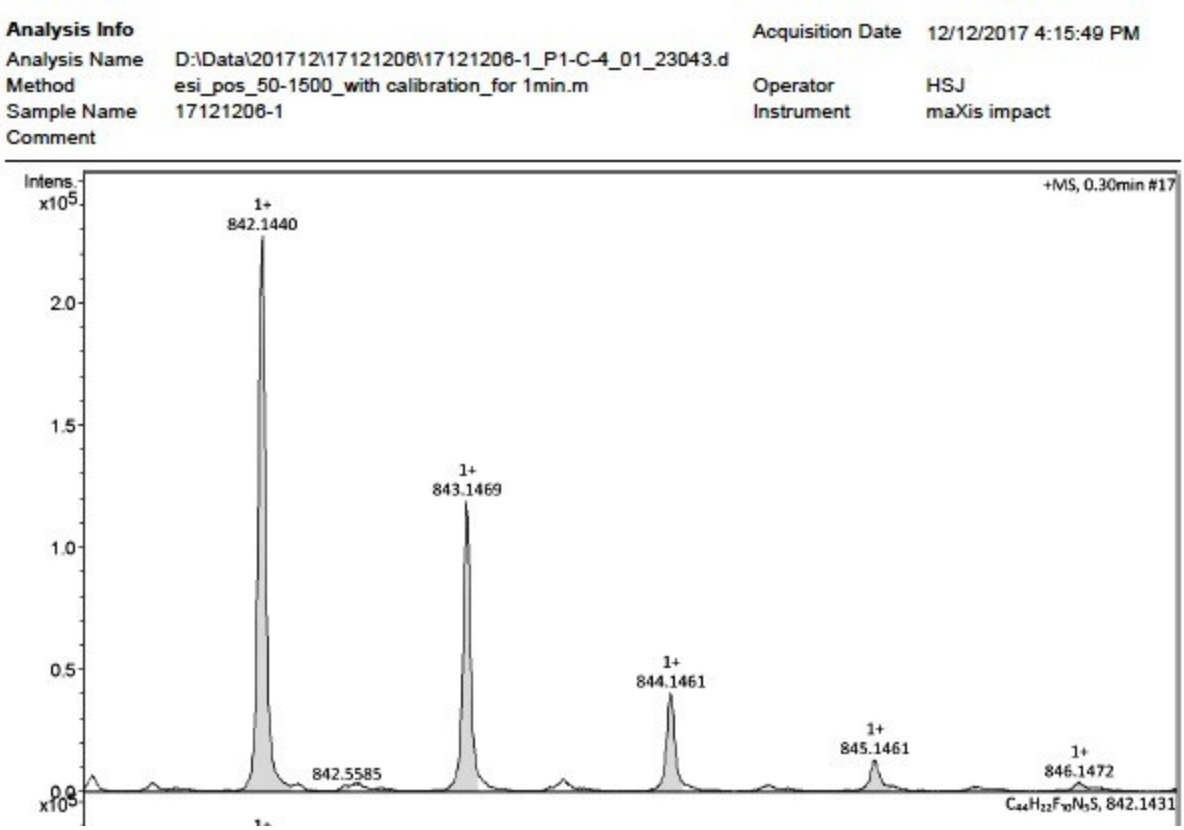

Fig. S2: HRMS Spectrum of F10C-PTZ dyad.

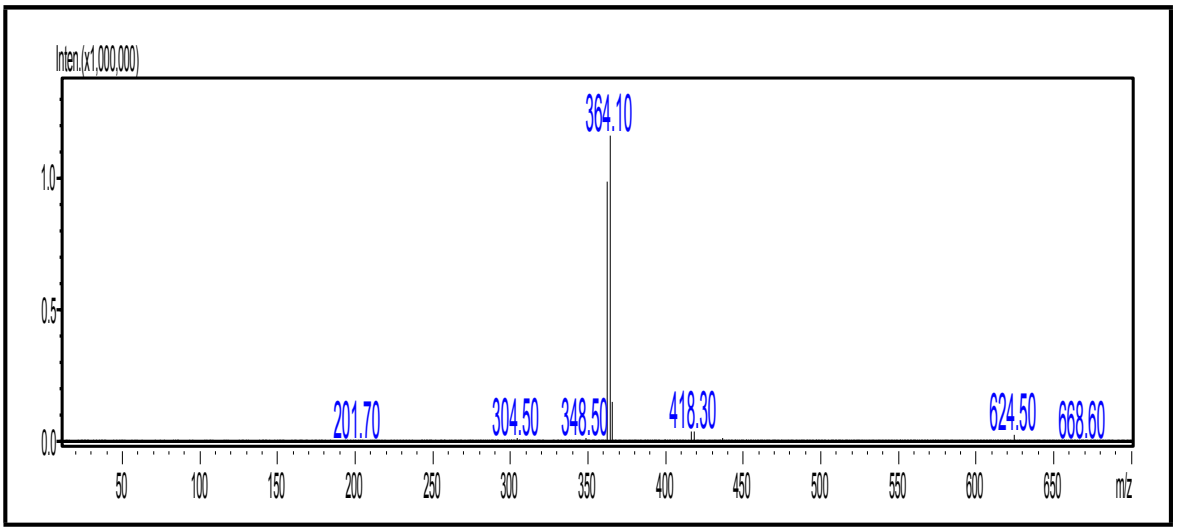

Fig. S3: ESI-MS Spectrum of DPQ-Br (6-bromo-2,3-di(pyridin-2-yl)quinoxaline).

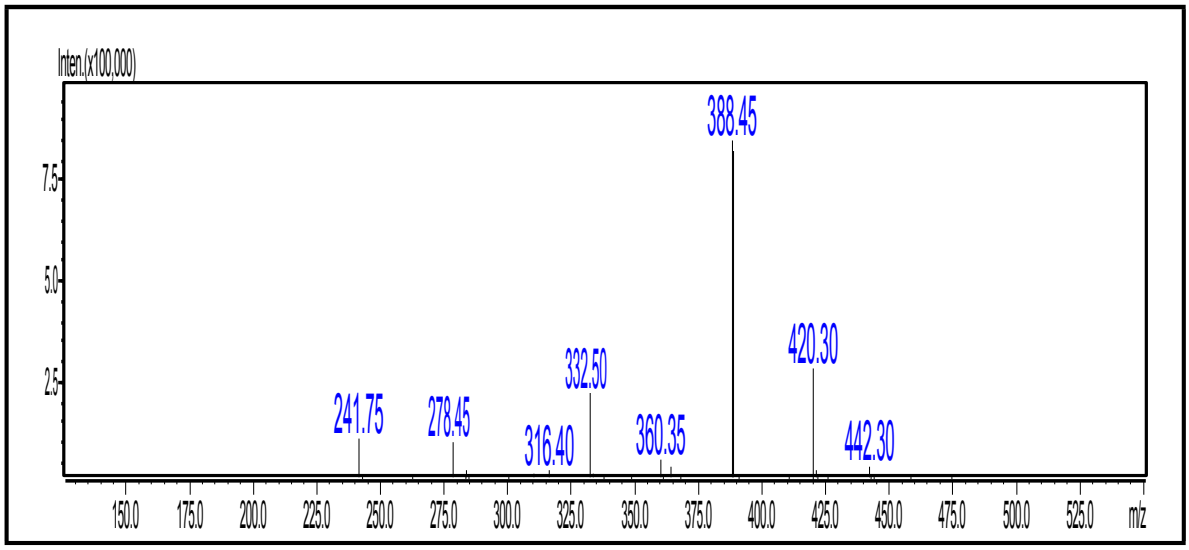

Fig. S4: ESI-MS Spectrum of DPQ-CHO (4-(2,3-di(pyridin-2-yl)quinoxalin-6-yl)benzaldehyde).

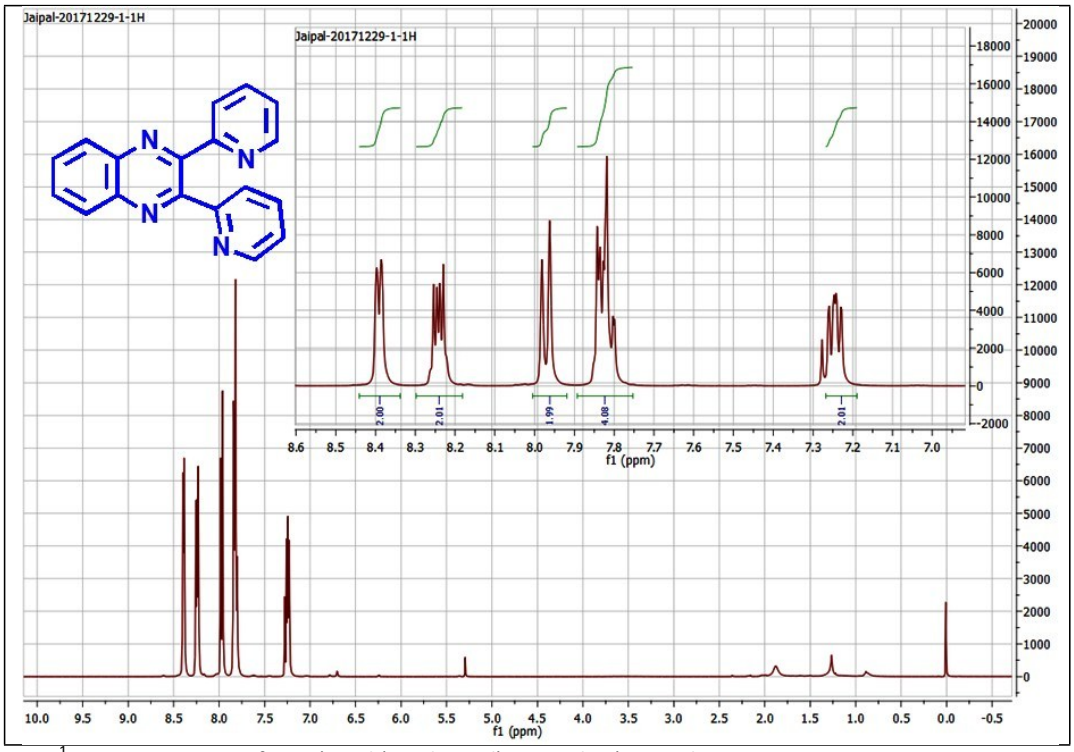

Fig. S5: ^{1}H -NMR spectrum of DPQ (2,3-di(pyridin-2-yl)quinoxaline) in $CDCl_3$

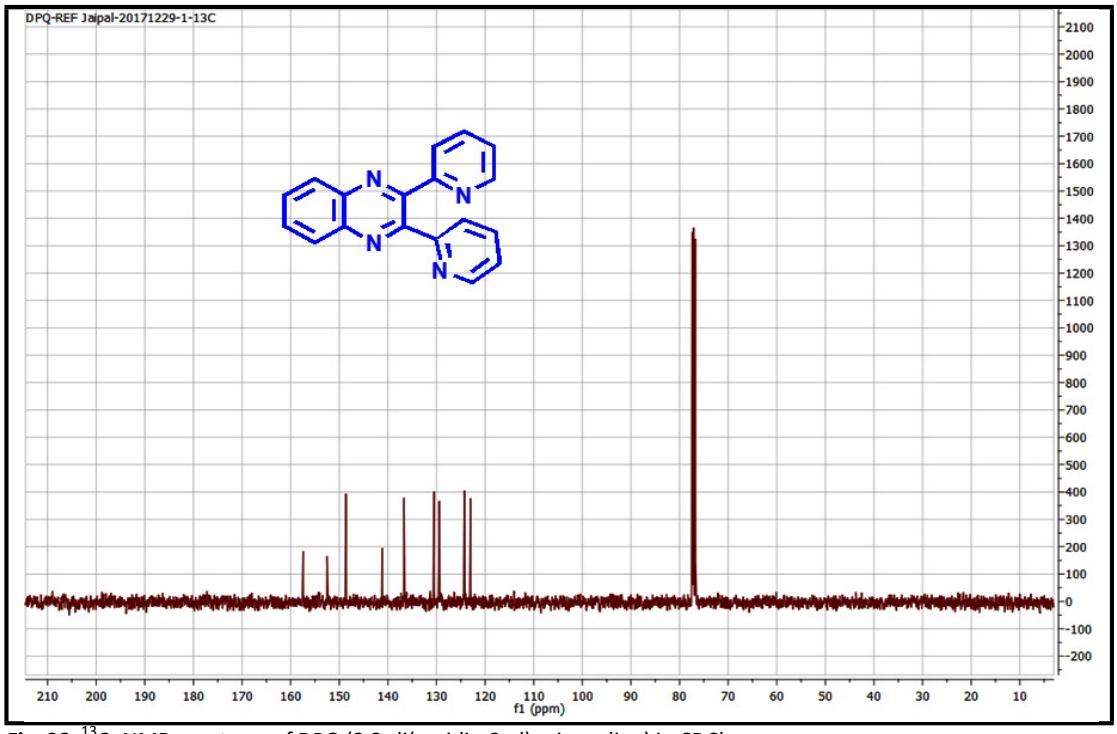

Fig. S6: ^{13}C -NMR spectrum of DPQ (2,3-di(pyridin-2-yl)quinoxaline) in $CDCl_3$

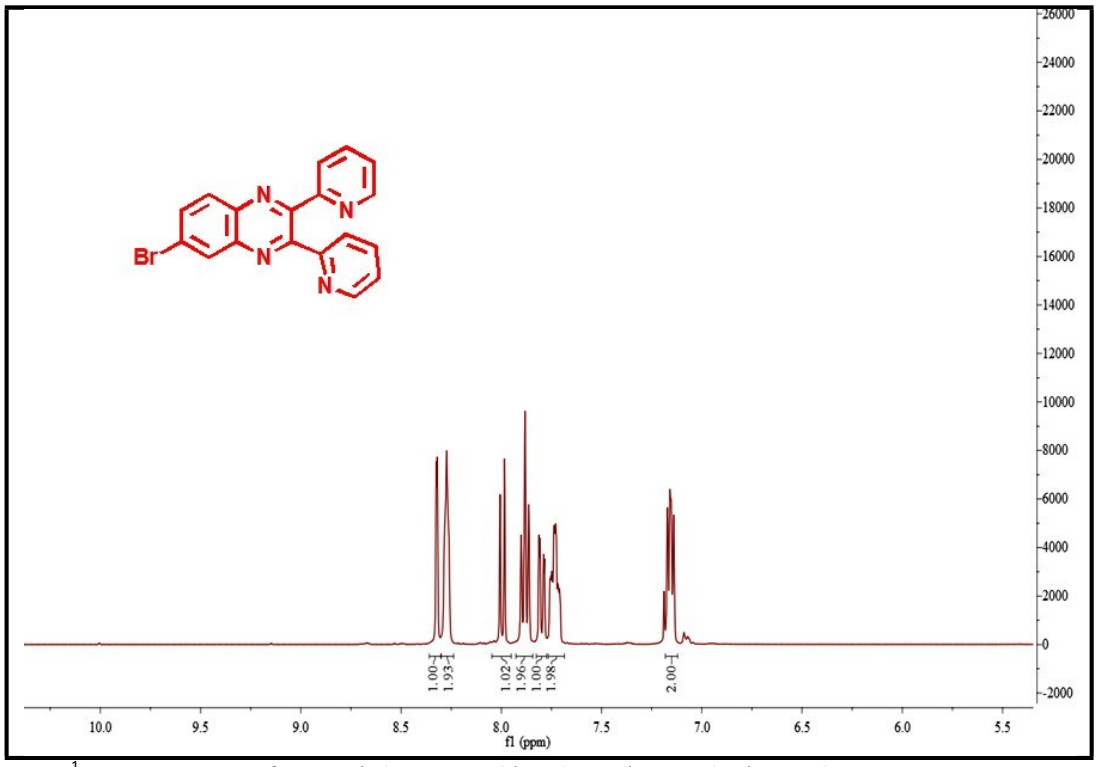

Fig. S7: ^{1}H -NMR spectrum of DPQ-Br (6-bromo-2,3-di(pyridin-2-yl)quinoxaline) in $CDCl_3$

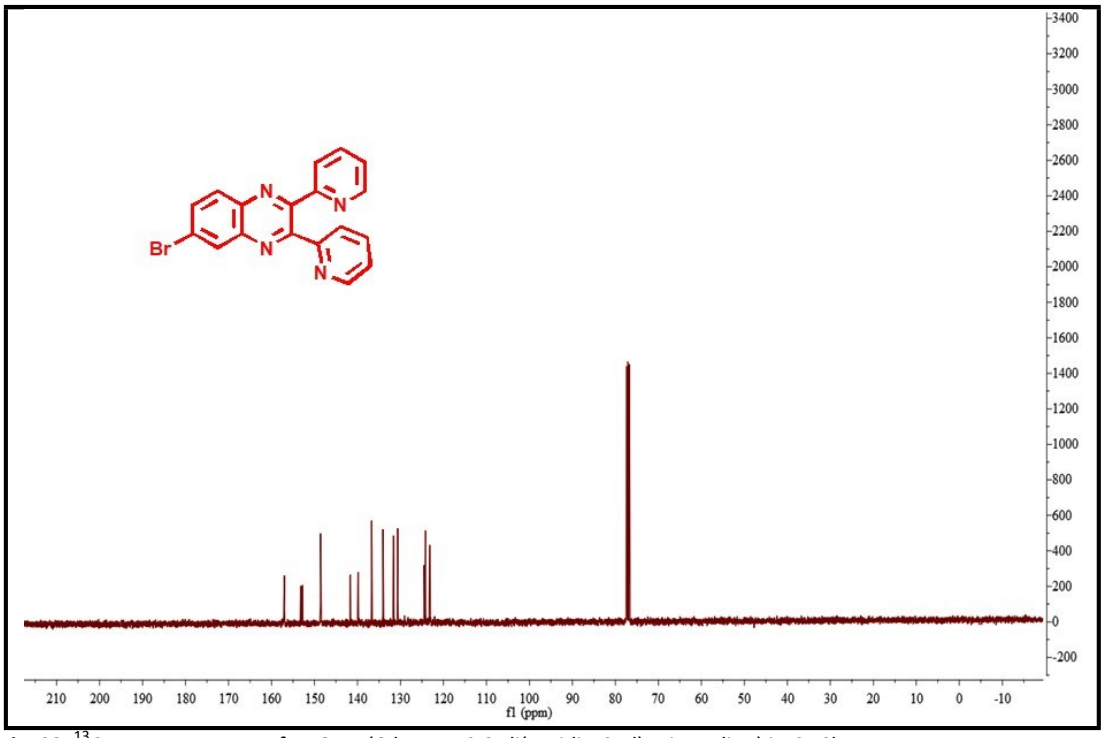

Fig. S8: ^{13}C -NMR spectrum of DPQ-Br (6-bromo-2,3-di(pyridin-2-yl)quinoxaline) in $CDCl_3$

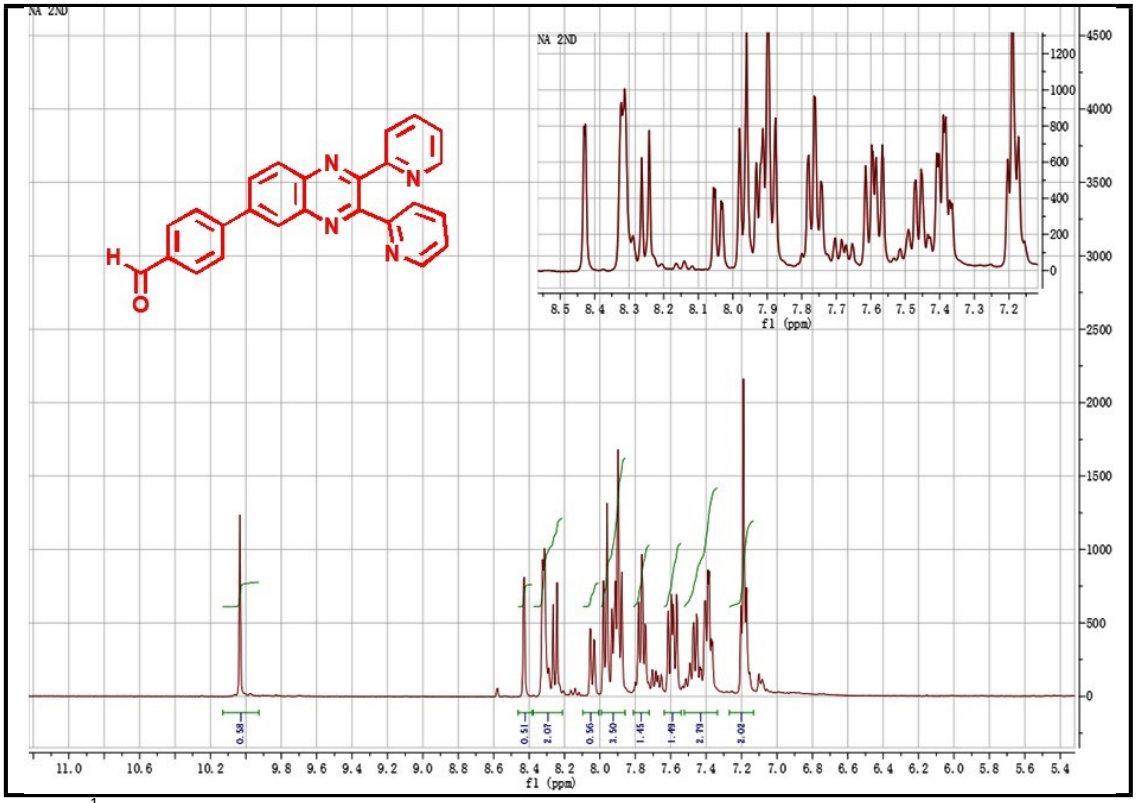

Fig. S9: ^{1}H -NMR spectrum of DPQ-CHO (4-(2,3-di(pyridin-2-yl)quinoxalin-6-yl)benzaldehyde) in $CDCl_3$

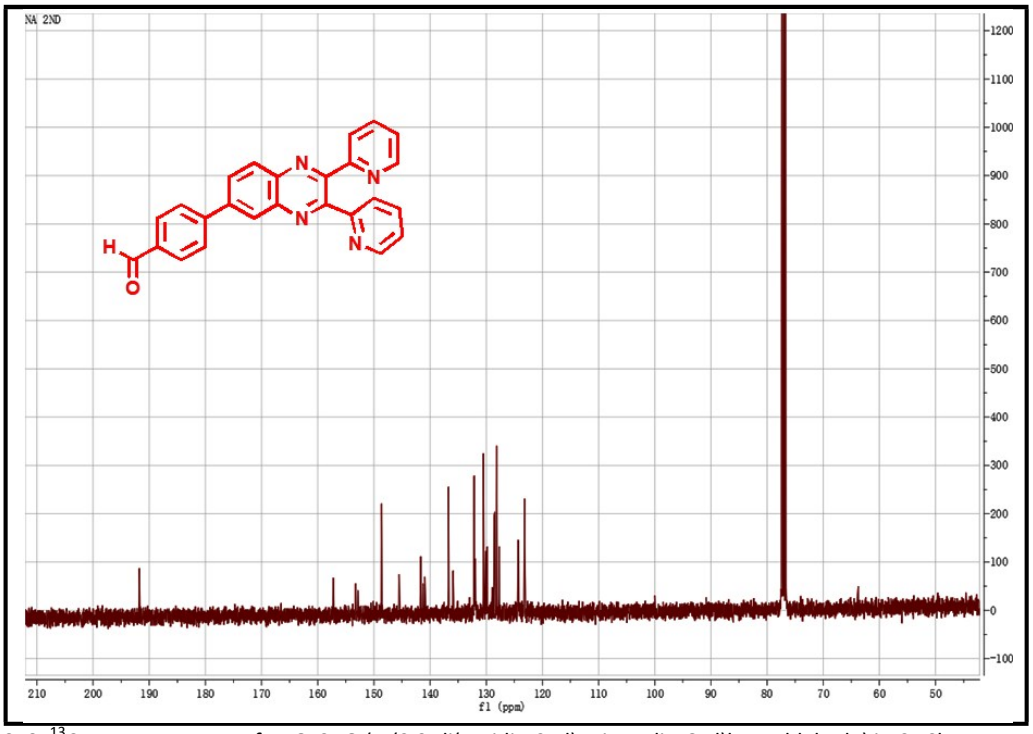

Fig. S10: ^{13}C -NMR spectrum of DPQ-CHO (4-(2,3-di(pyridin-2-yl)quinoxalin-6-yl)benzaldehyde) in $CDCl_3$

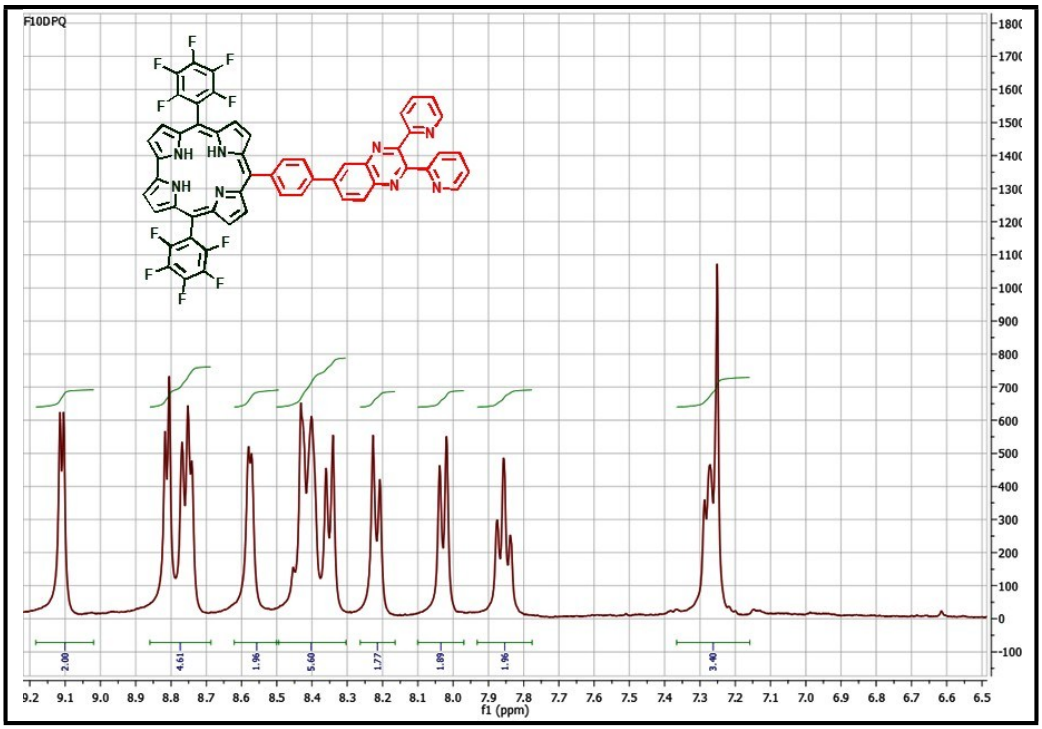

Fig. S11: ^{1}H -NMR spectrum of F10C-DPQ dyad in $CDCl_3$

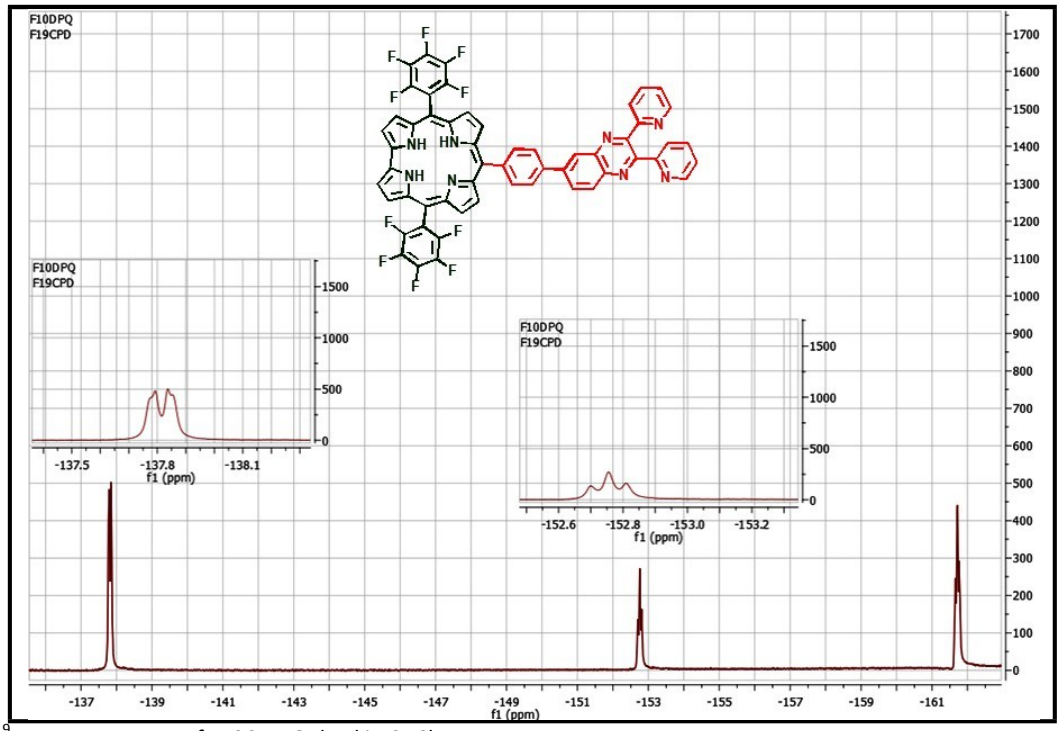

Fig. S12: ^{19}F -NMR spectrum of F10C-DPQ dyad in $CDCl_3$

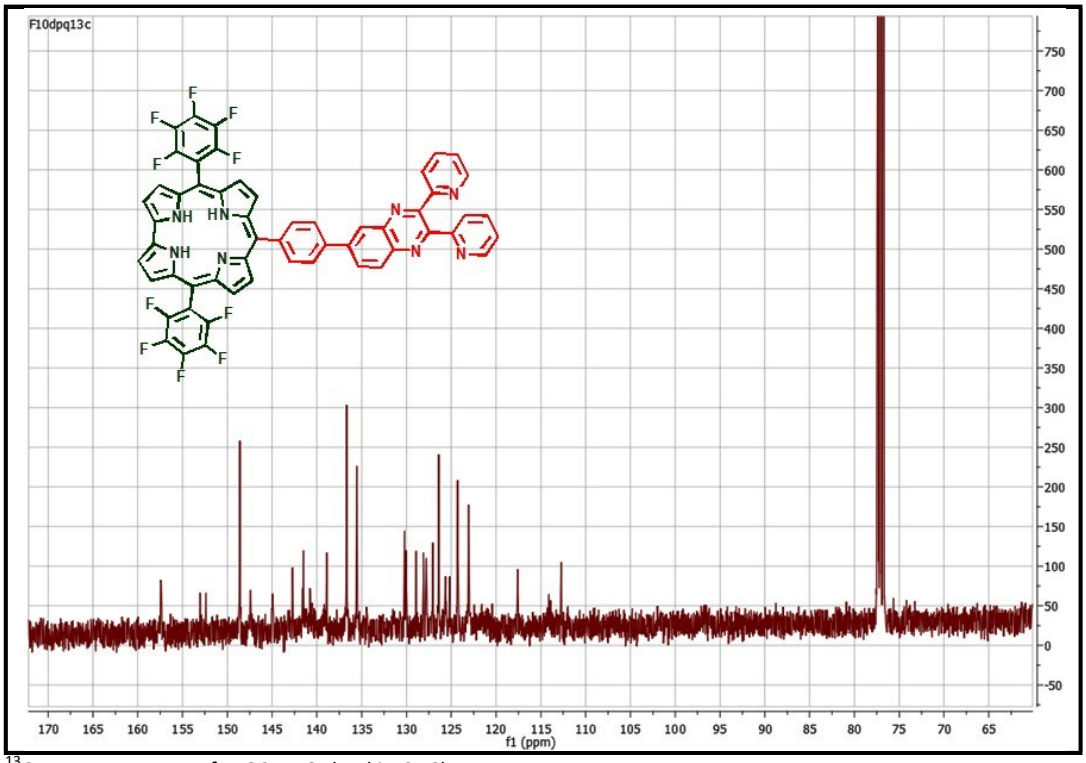

Fig. S13: ^{13}C -NMR spectrum of F10C-DPQ dyad in $CDCl_3$

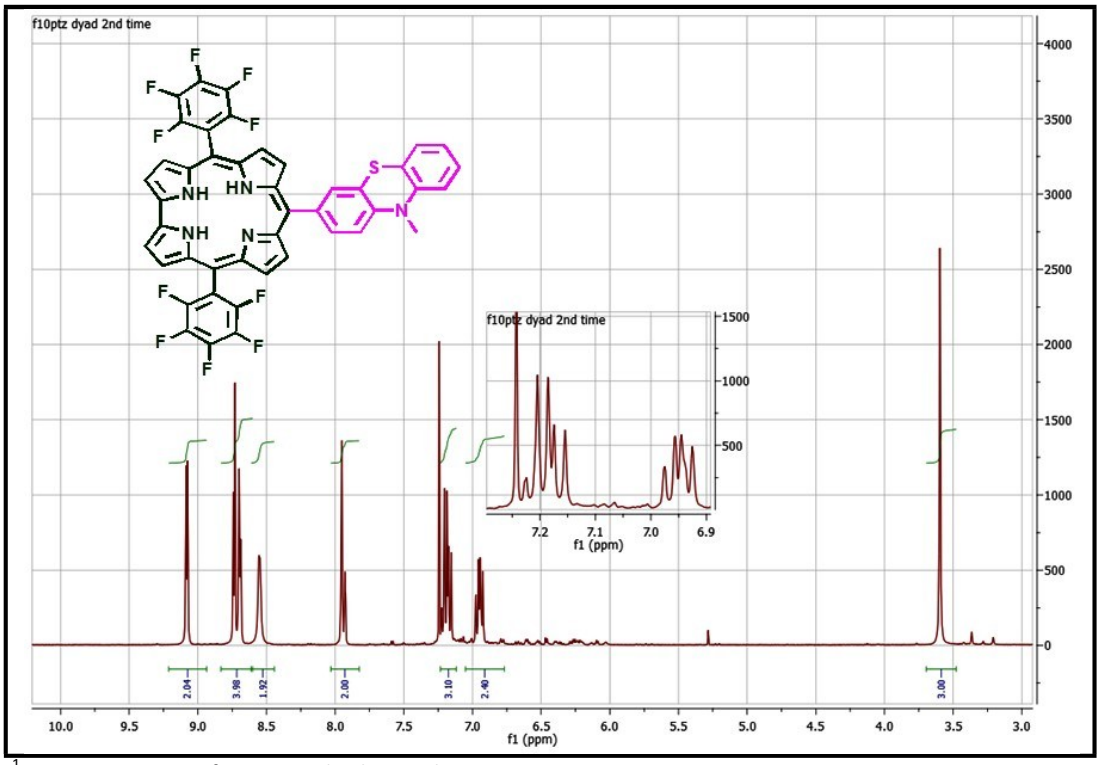

Fig. S14: ^{1}H -NMR spectrum of F10C-PTZ dyad in $CDCl_3$

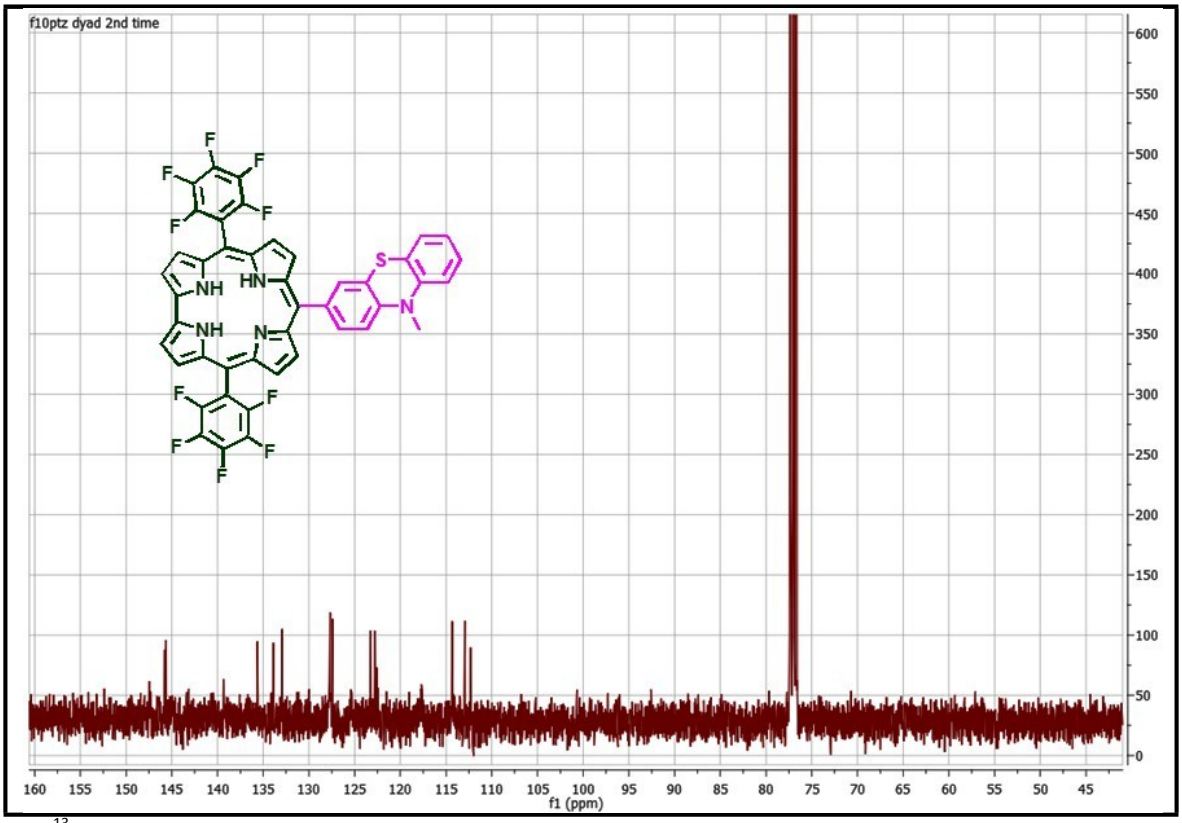

Fig. S15: ^{13}C -NMR spectrum of F10C-PTZ dyad in $CDCl_3$

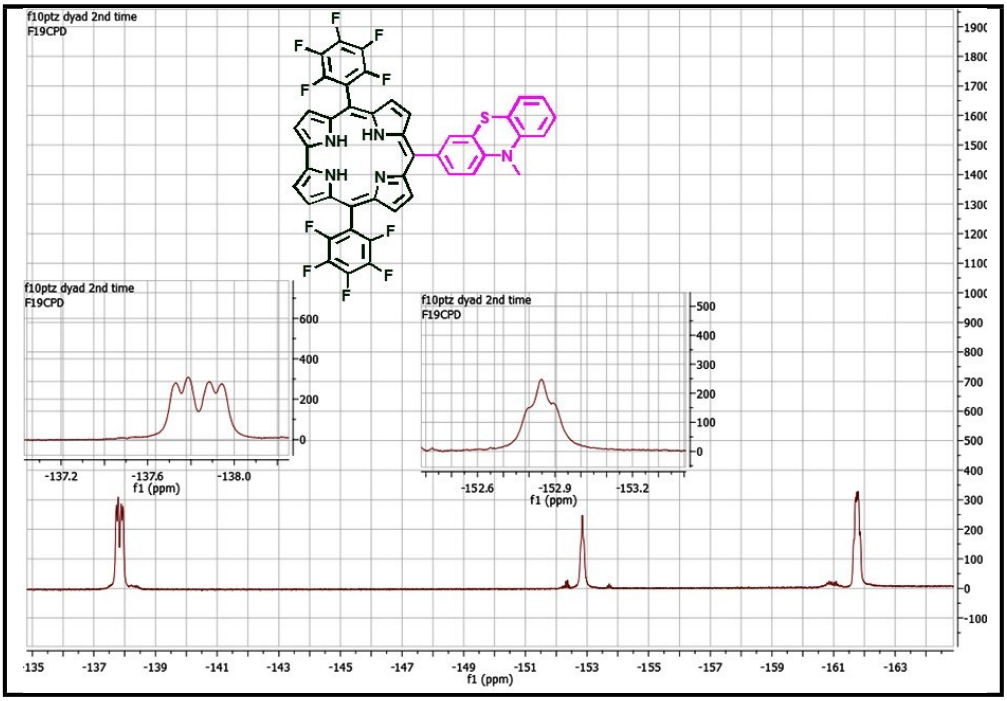

Fig. S16: ^{19}F -NMR spectrum of F10C-PTZ dyad in $CDCl_3$

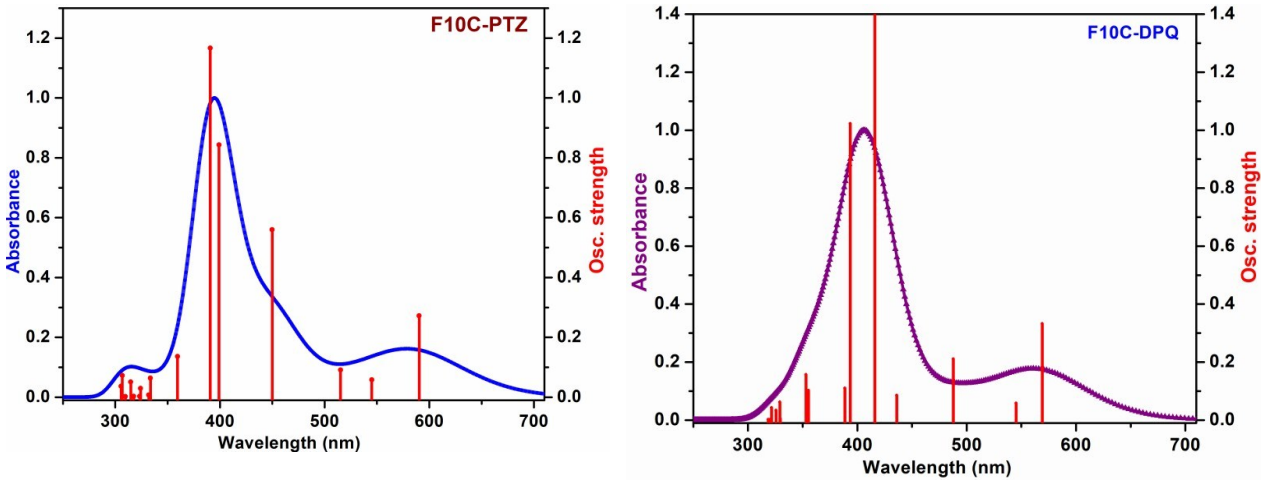

Fig. S17: Theoretical absorption spectra of F10C-PTZ and F10C-DPQ dyads by using B3LYP method PCM model in dichloromethane solvent.

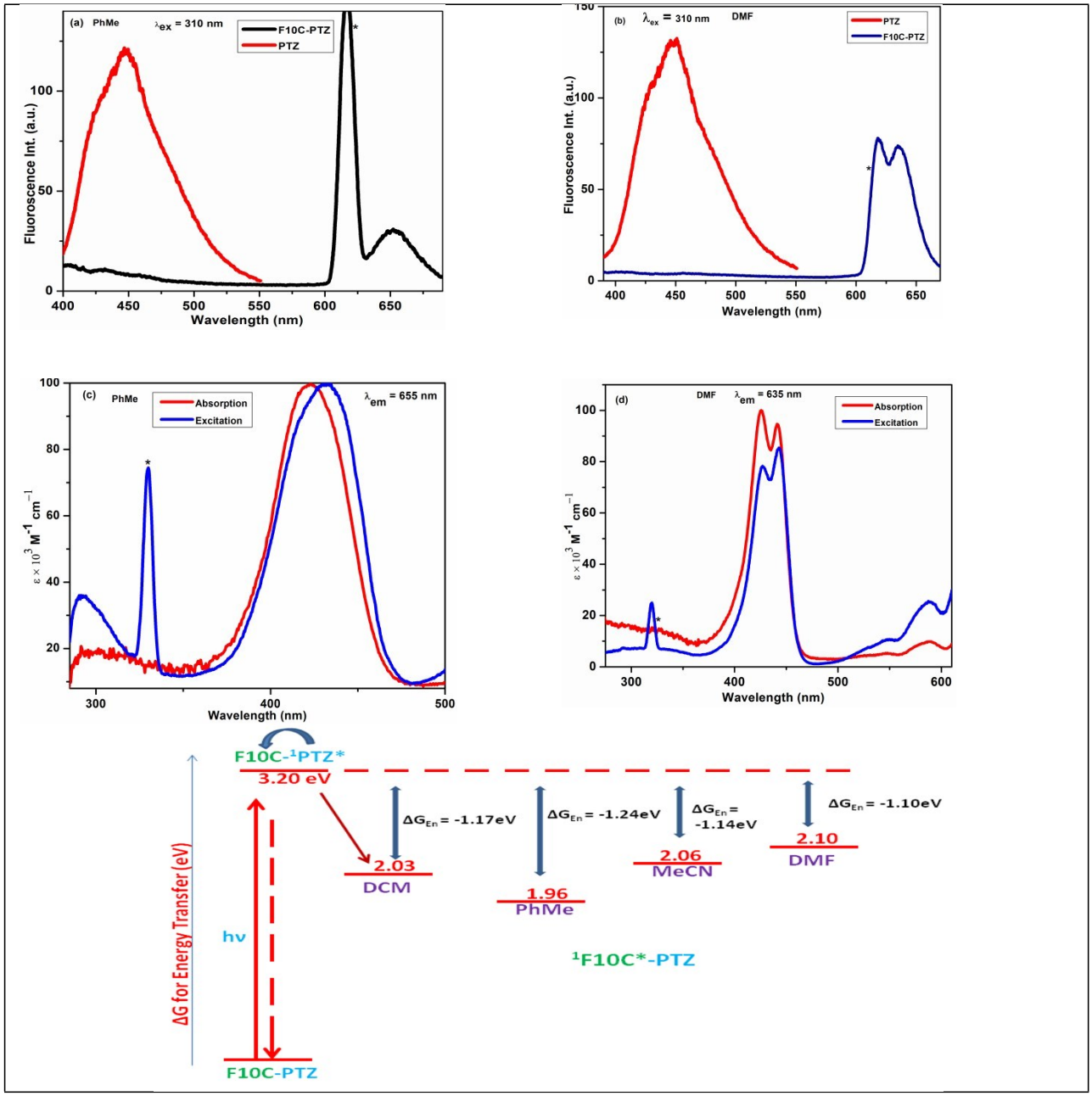

Fig. S18: Emission spectra (a) & (b) and Excitation spectra (c) & (d) of the F10C-PTZ dyad in toluene and DMF, free energy change for energy transfer in different solvents were shown in bottom.

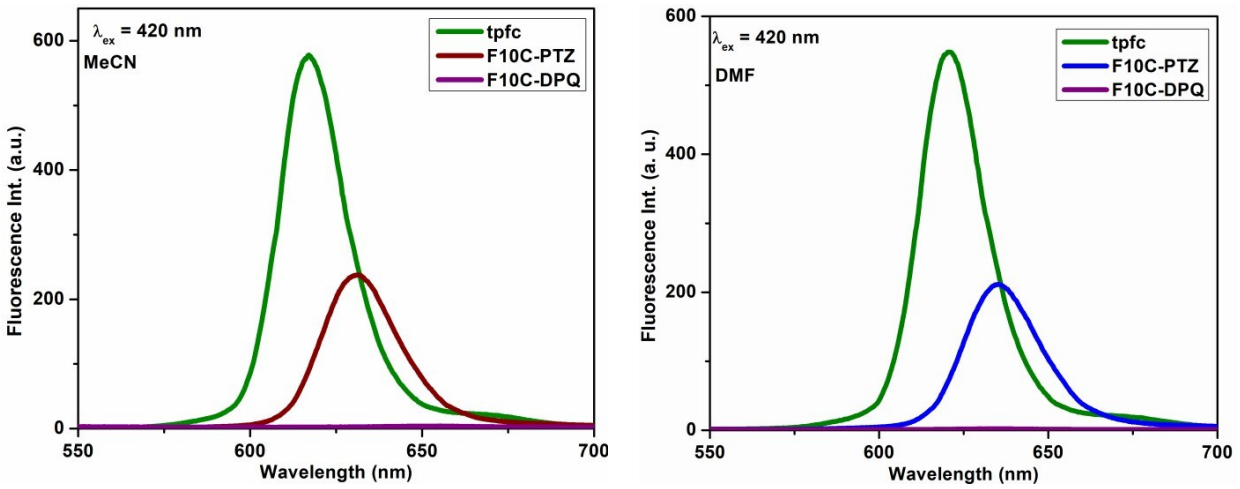

Fig. S19: Emission spectra of F10C-PTZ and F10C-DPQ dyads in Acetonitrile and dimethylformamide (λ_{ex} = 420 nm and O.D. of all the samples were 0.05).

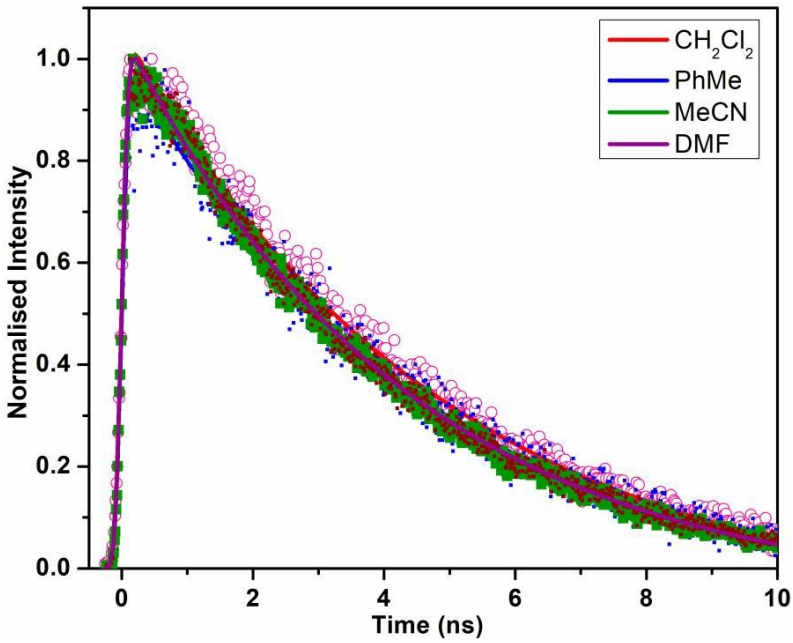

Fig. S20: Fluorescence decay of the pristine corrole (5,10,15tris(pentafluorophenyl)corrole) in four different solvents (λ_{ex} = 420 nm and λ_{em} monitored at their respective wavelengths in different solvents.

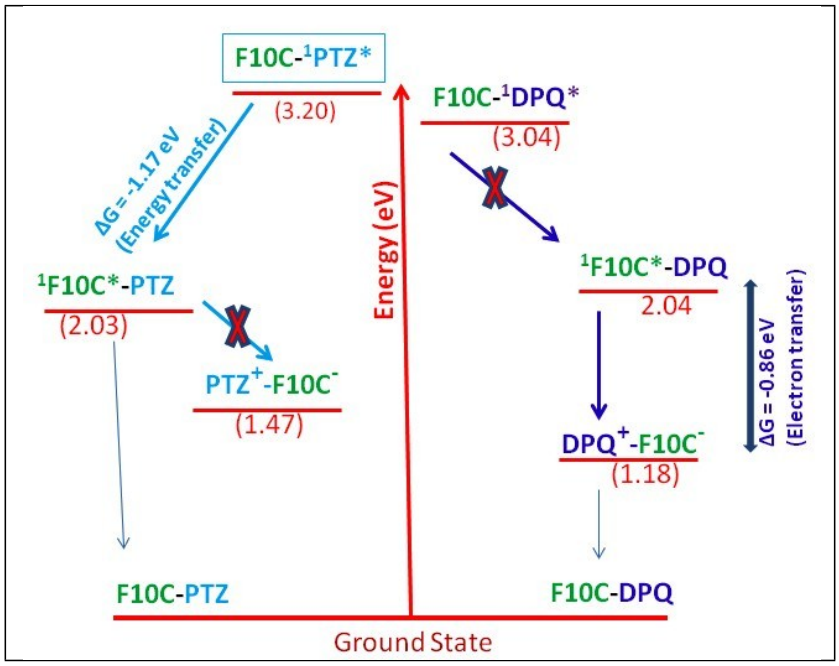

Fig. S21: Energy level diagram of the both the dyads in CH_2Cl_2. the singlet state energy of the F10C-DPQ was assumed to 3.04 eV , due to lack of emission of pristine DPQ, we cannot overlap the absorption and emission of the DPQ, but we have estimated the value according to previous reports reference - 22 in the main text.