Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Design and synthesis of solution processable green fluorescent D-π-A dyads for OLED applications

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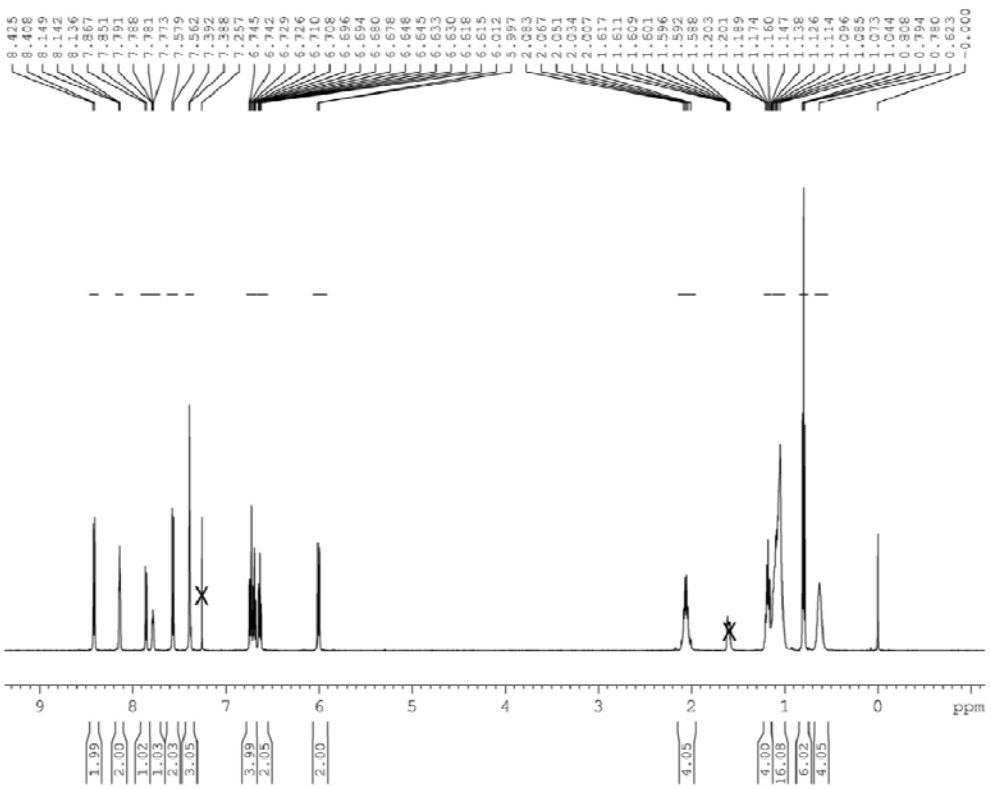

Fig. S1 ^{1}H NMR spectrum of the dyad **1** in $CDCl_3$.

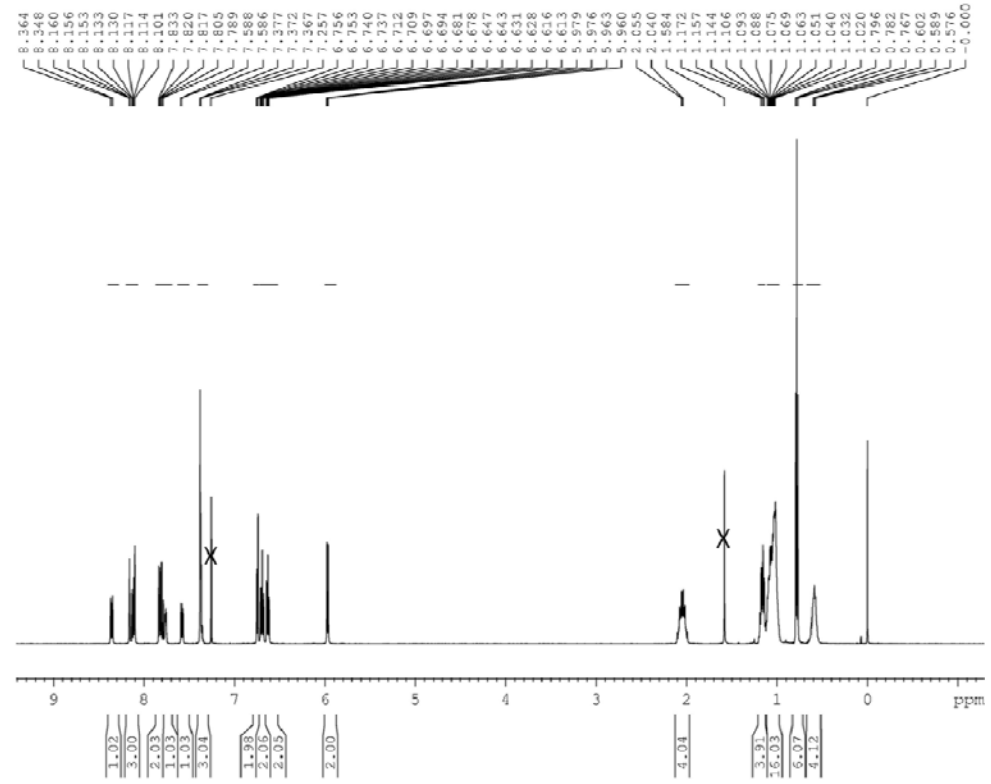

Fig. S2 ^{1}H NMR spectrum of the dyad **2** in $CDCl_3$.

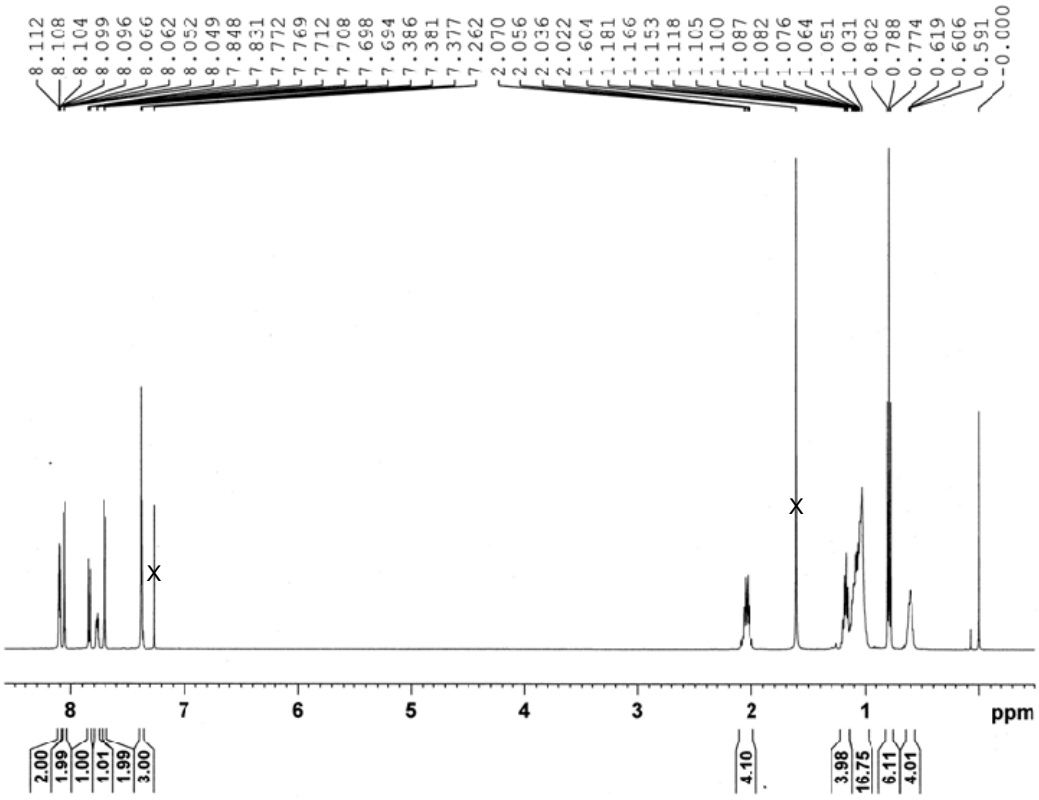

Fig. S3 ^{1}H NMR spectrum of ***p*-FOArBr** in $CDCl_3$.

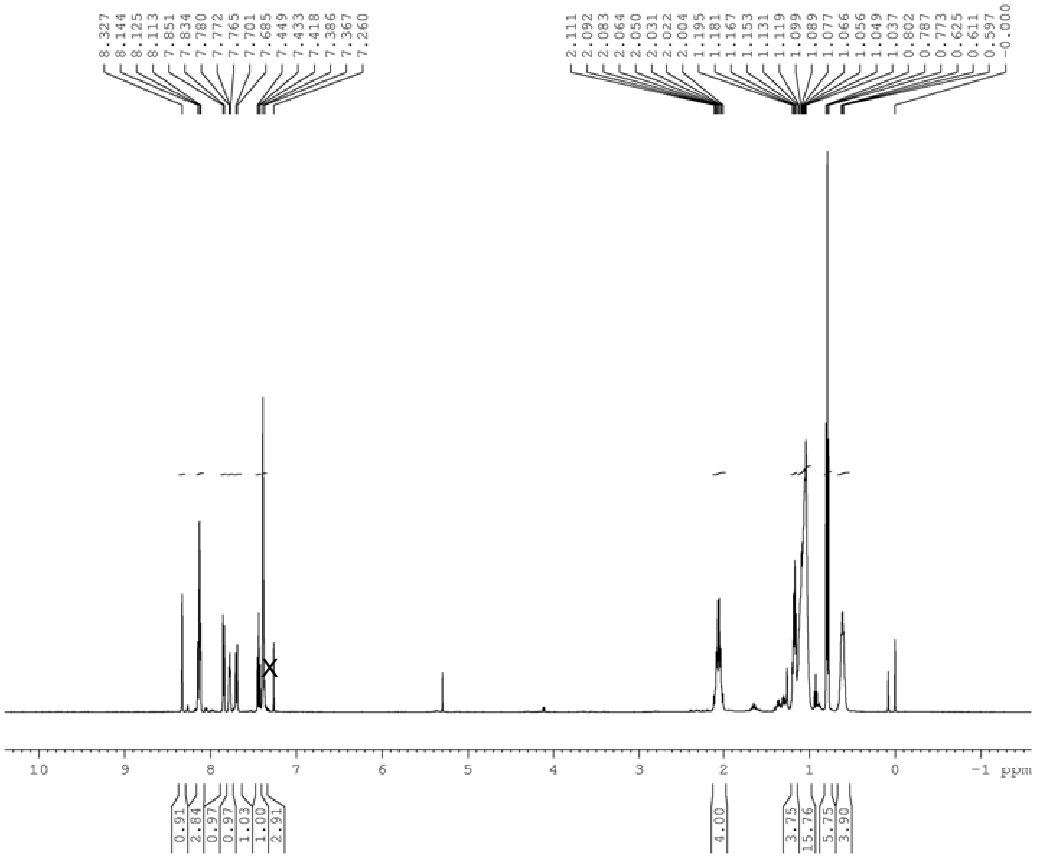

Fig. S4 ^{1}H NMR spectrum of ***m*-FOArBr** in $CDCl_3$.

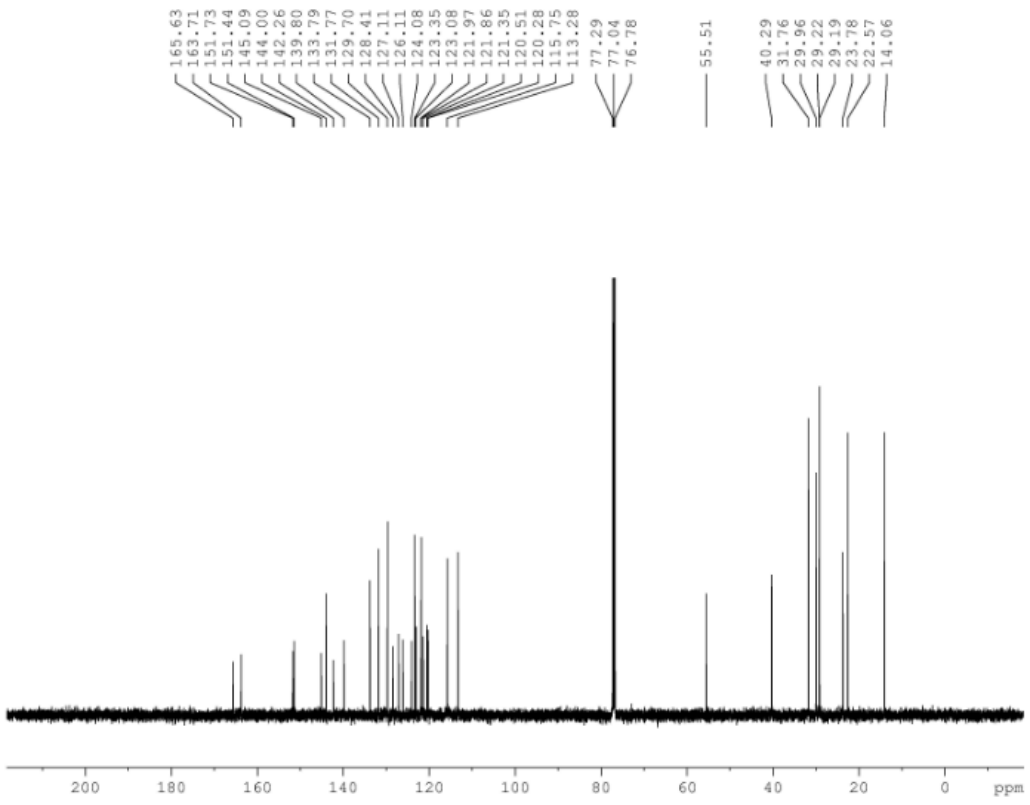

Fig. S5 ^{13}C NMR spectrum of the dyad **1** in $CDCl_3$.

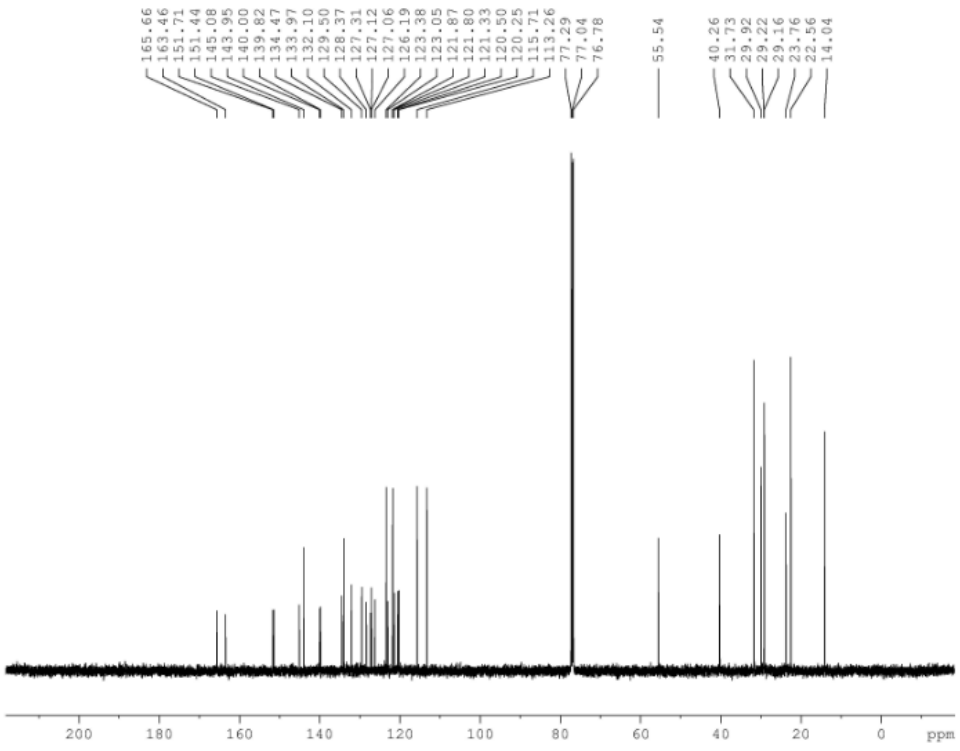

Fig. S6 ^{13}C NMR spectrum of the dyad **2** in $CDCl_3$.

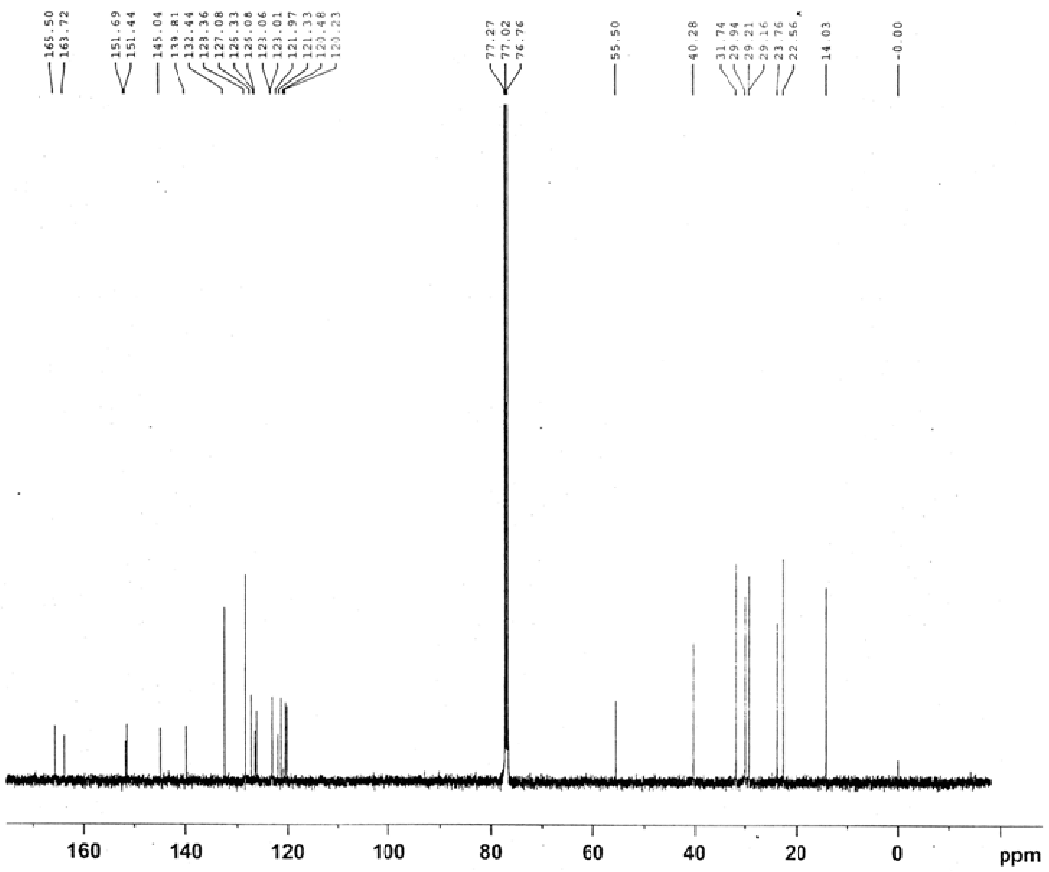

Fig. S7 ^{13}C NMR spectrum of ***p*-FOArBr** in $CDCl_3$.

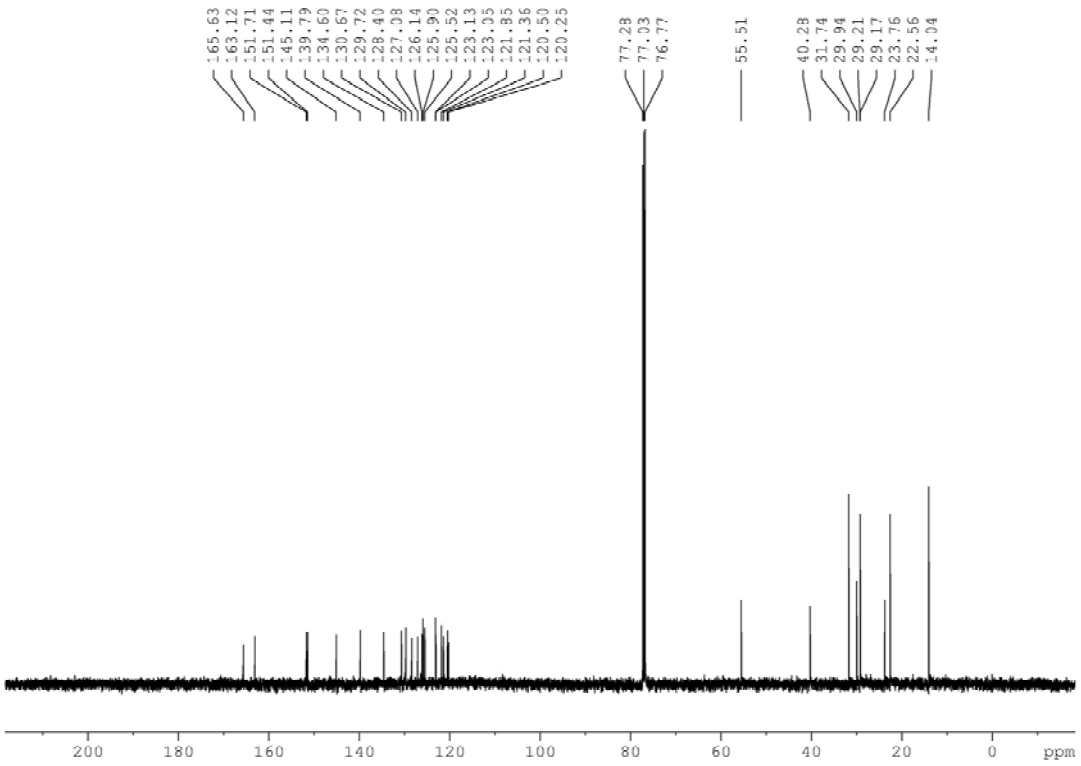

Fig. S8 ^{13}C NMR spectrum of ***m*-FOArBr** in $CDCl_3$.

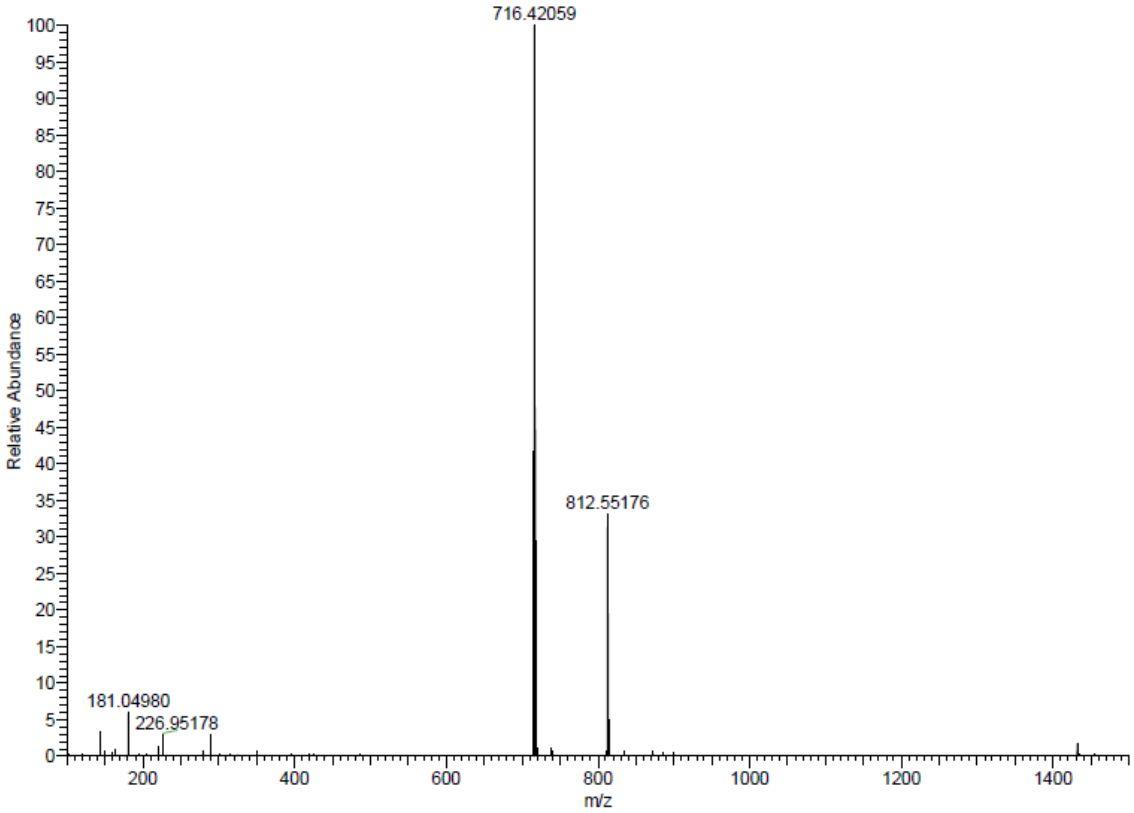

Fig. S9 ESI mass spectrum of the dyad **1**.

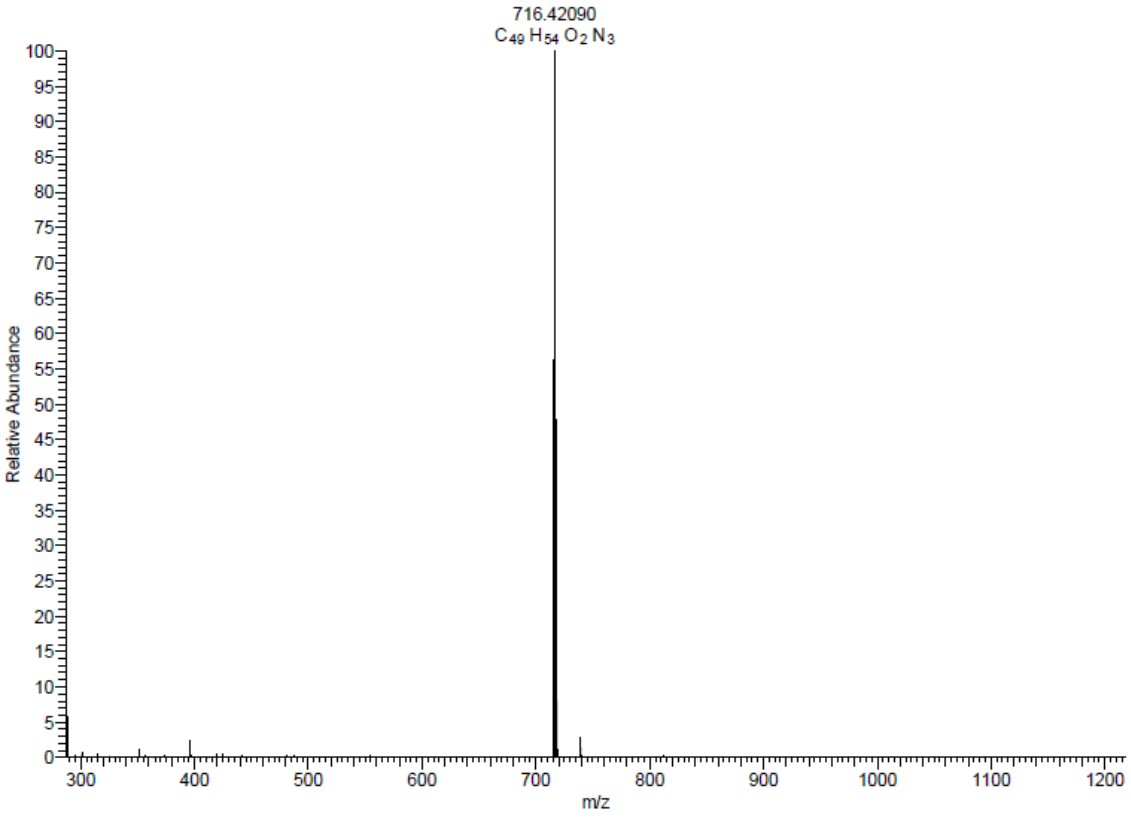

Fig. S10 ESI mass spectrum of the dyad **2**.

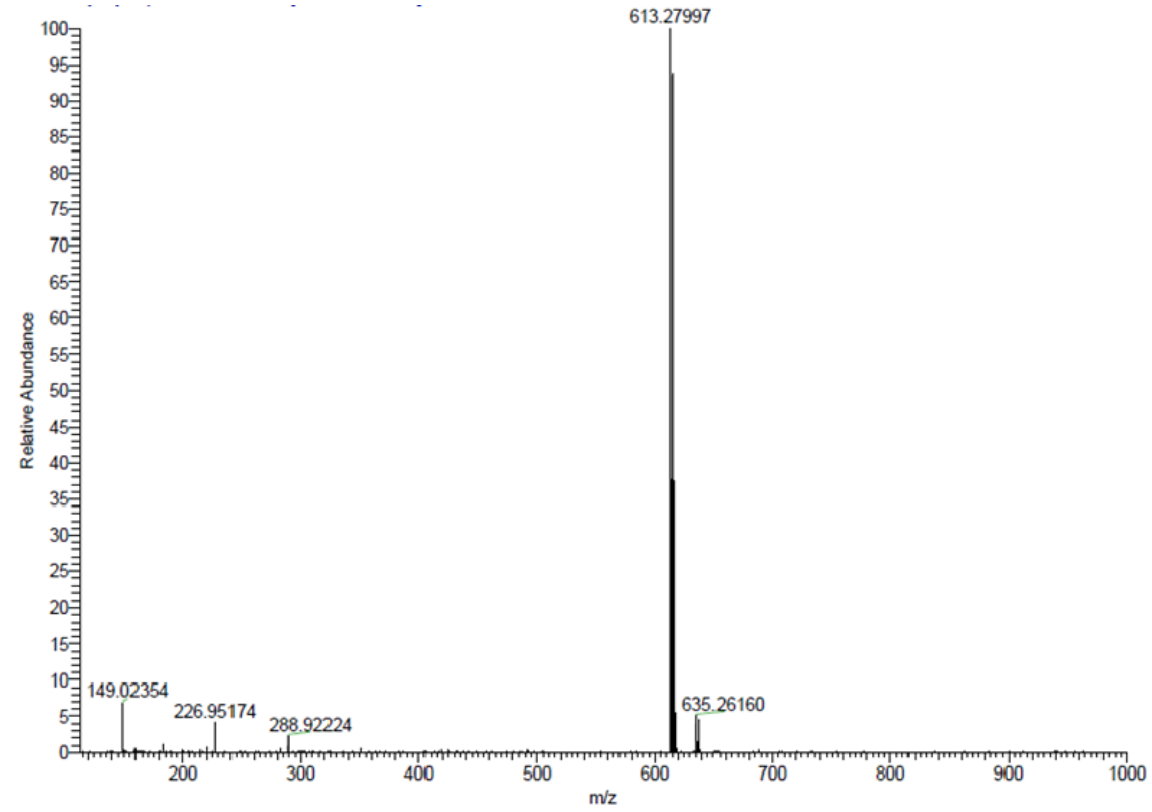

Fig. S11 ESI mass spectrum of ***p*-FOArBr**.

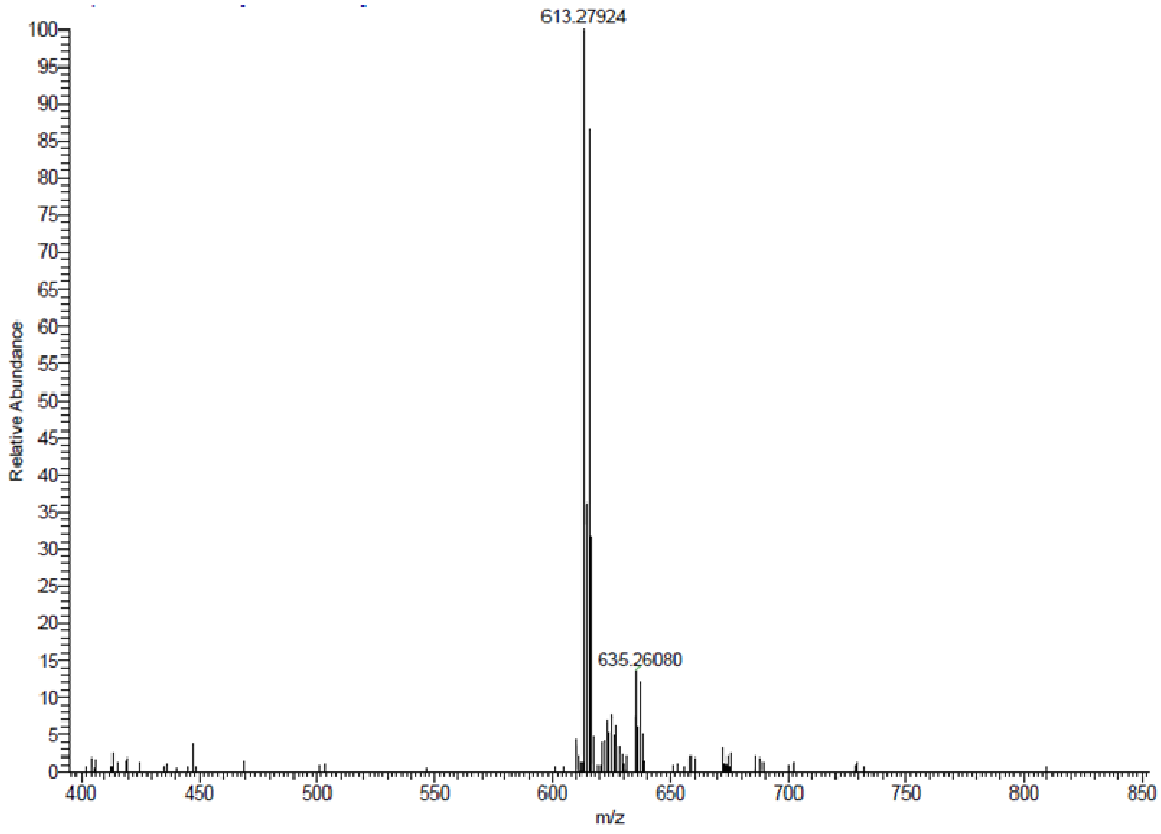

Fig. S12 ESI mass spectrum of ***m*-FOArBr**.

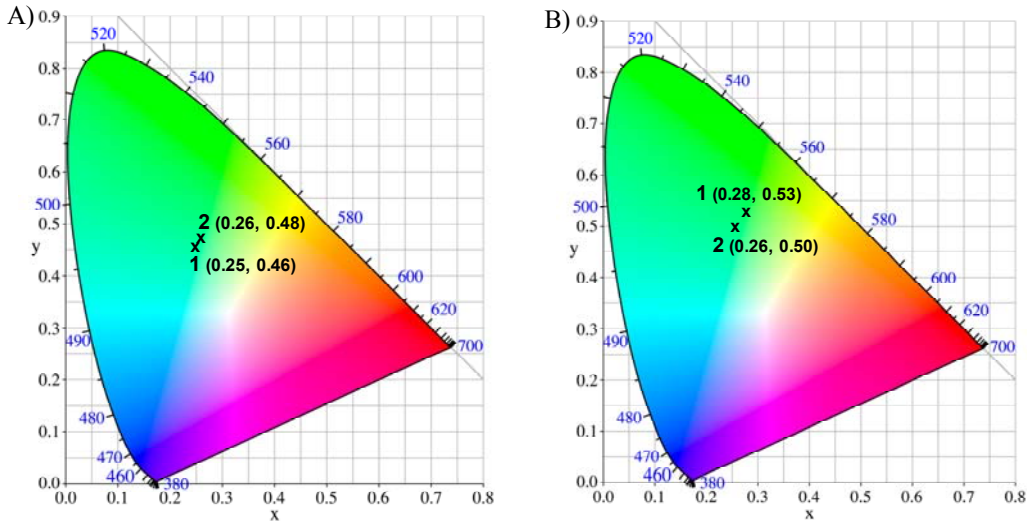

Fig. S13 CIE chromaticity diagram of the dyads **1** and **2** corresponding to the emission spectra in (A) toluene and (B) thin film state.

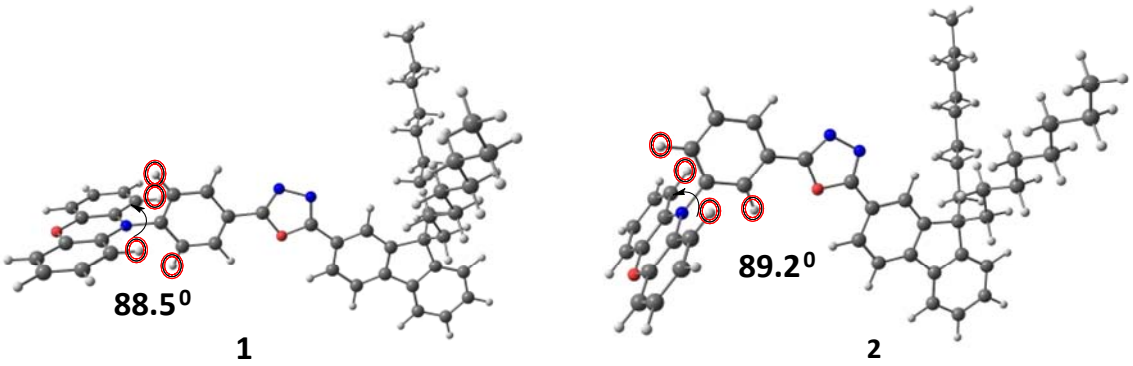

Fig. S14 Ground state optimized geometries of the dyads **1** and **2**. The hydrogen atoms responsible for the twisted configuration are highlighted in red circles.

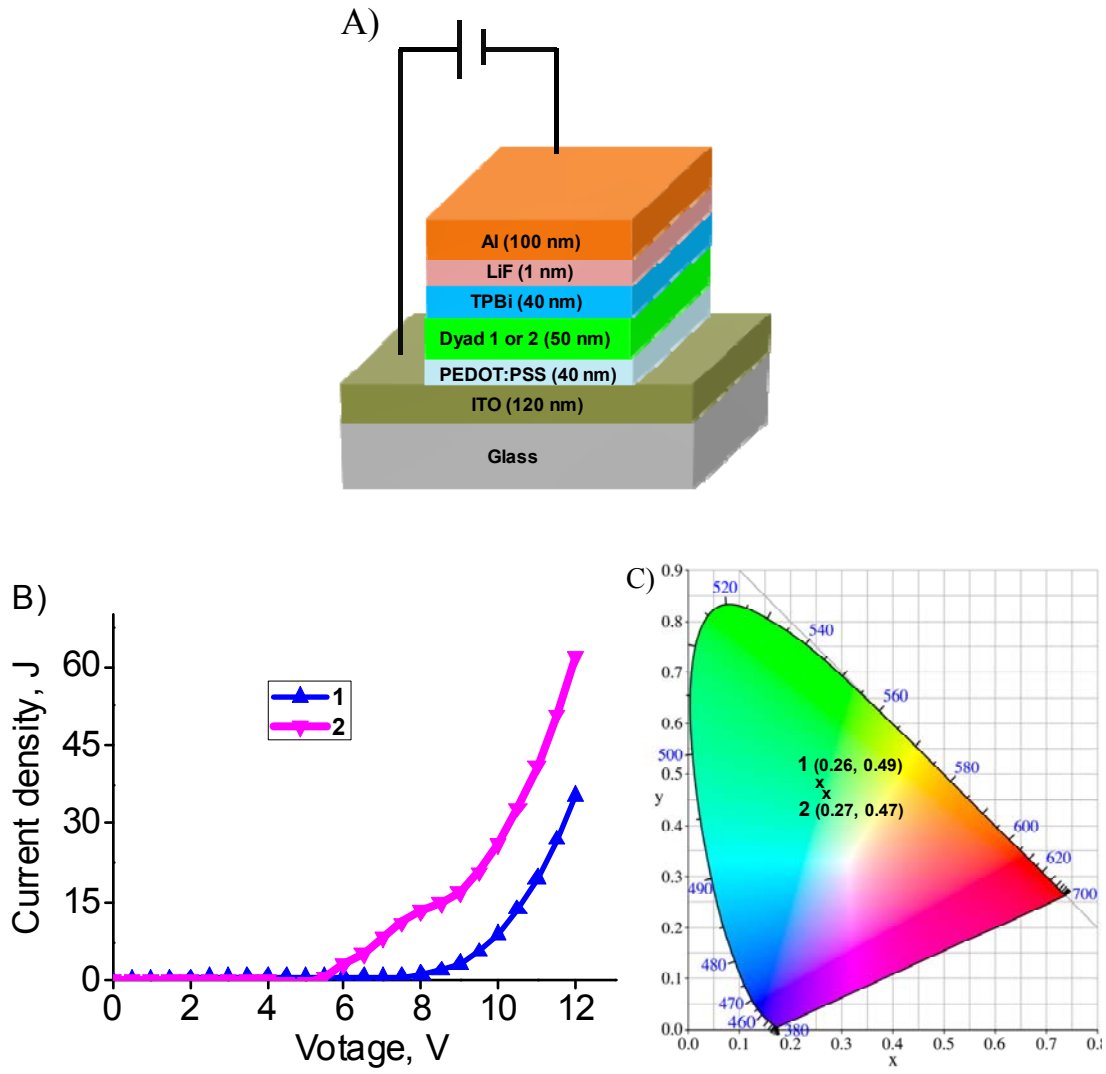

Fig. S15 Device structure (A), current density-voltage plot (B) and CIE chromaticity diagram (C) of the OLEDs fabricated using the dyads **1** and **2**.

Table S1 Absorption and emission properties of dyad **1** in different solvents. [a]

Solvents	ε	n	Δf	λ_a (nm)	ν_a (cm^{-1})	λ_f (nm)	ν_f (cm^{-1})	ν_a - ν_f (cm^{-1})
Cyclohexane	2.02	1.43	0.005	327,390	30581.0	465	21505.4	9075.6
Toluene	2.38	1.49	0.013	328, 390	30487.8	505	19801.9	10685.8
DCM	9.10	1.42	0.220	328, 380	30487.8	562	17793.6	12694.2
Acetone	21.00	1.36	0.286	328, 373	30487.8	598	16722.4	13765.4
Acetonitrile	37.50	1.35	0.303	326, 372	30674.8	620	16129.0	14545.7

[a]Average of more than three independent experiments, ε: dielectric constant, n: refractive index, Δf: solvent polarity parameter, λ_a: absorption wavelength, ν_a: wave number corresponds to absorption maximum, λ_f: fluorescence wavelength, ν_a: wave number corresponds to fluorescence maximum.

Table S2 Absorption and emission properties of dyad **2** in different solvents.[a]

Solvents	Δf	λ_{abs} (nm)	ν_a (cm^{-1})	λ_f (nm)	ν_f (cm^{-1})	ν_a - ν_f (cm^{-1})
Cyclohexane	0.005	328,345	30487.8	465	21505.38	8982.4
Toluene	0.013	330, 345	30303.0	522	19157.09	11145.9
DCM	0.220	329, 343	30395.1	575	17391.30	13003.8
Acetone	0.286	328, 341	30487.8	610	16393.44	14094.4
Acetonitrile	0.303	326, 340	30674.8	625	16000.00	14674.8

[a]Average of more than three independent experiments, Δf: solvent polarity parameter, λ_a: absorption wavelength, ν_a: wave number corresponds to absorption maximum, λ_f: fluorescence wavelength, ν_a: wave number corresponds to fluorescence maximum.

Table S3 Comparison of properties of the present dyads with previously reported D-A type emitters.

Sl. No	Publication	D-A Type	Thermal stability and device performance
1	Current Paper	Phenoxazine - Oxadiazole	Thermally stable up to 425 °C, excellent solution process-ability, film morphologies and un-doped OLED device performance based on dyad **1**: L_{max} = 1751 cd/ m^2, λ_{ems} = 504 nm, CIE (0.26, 0.49).
2	*Photochem. Photobiol. Sci.*, 2014, **13**, 342 – 357	Anthracene - Oxadiazole	Thermally stable up to 364 °C and un-doped OLED device performance based on dyad **8A**: L_{max} = 1284 cd/ m^2, λ_{ems} = 485 nm, V_{onset} = 3V.
3	*New J. Chem.*, 2014, **38**, 2368 – 2378	Indolo[3,2-b]carbazole - Dimesitylboron	Thermally stable up to 210 °C and un-doped OLED device performance based on dyad **A**: L_{max} = 5634 cd/ m^2; λ_{ems} = 472 nm; V_{onset} = 6.1 V
4	*Chem. Asian J.* 2013, **8**, 2111 – 2124	Pyrene - Pyrenoimidazole	Thermally stable up to 500 °C and doped blue OLED device performance based on dyad **4c**: L_{max} = 2980 cd/ m^2; CIE (0.156, 0.135)
5	*Chem. Asian J.* 2010, **5**, 2093 – 2099	Triphenylamine - Benzimidazole	Thermally stable up to 531 °C and un-doped blue OLED device performance based on dyad **A**: L_{max} = 4448 cd/ m^2; V_{onset} = 3.5 V; CIE (0.17, 0.07)
6	*J. Mater.* Chem., 2009, **19**, 6172–6184	Anthracene – Oxadiazole	Thermally stable up to 460 °C and un-doped OLED device performance based on dyad **5**: L_{max} = 1996 cd/ m^2, λ_{ems} = 535 nm, V_{onset} = 4V.