Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis, Photophysical and Electrochemical Studies of Acridone-Amine based Donor-Acceptors for Hole Transport Materials

Abbreviations:

The following abbreviations are used throughout the manuscript and supporting information dipalladium-tris(dibenzylideneacetone), $Pd_2(dba)_3$; 2-dicyclohexylphoshpino-2`,6`-dimethylbiphenyl, SPhos; sodium-tert-butoxide, t-BuONa; Calculated, calcd; Necular magnetic resonance, NMR; MALDI-TOF; Fourier transform infrared, FT-IR; Cyclic voltammetry, CV; Differential Pulse voltammetry, DPV.

1) ^{1}H and ^{13}C NMR Spectra of compounds (1-7)

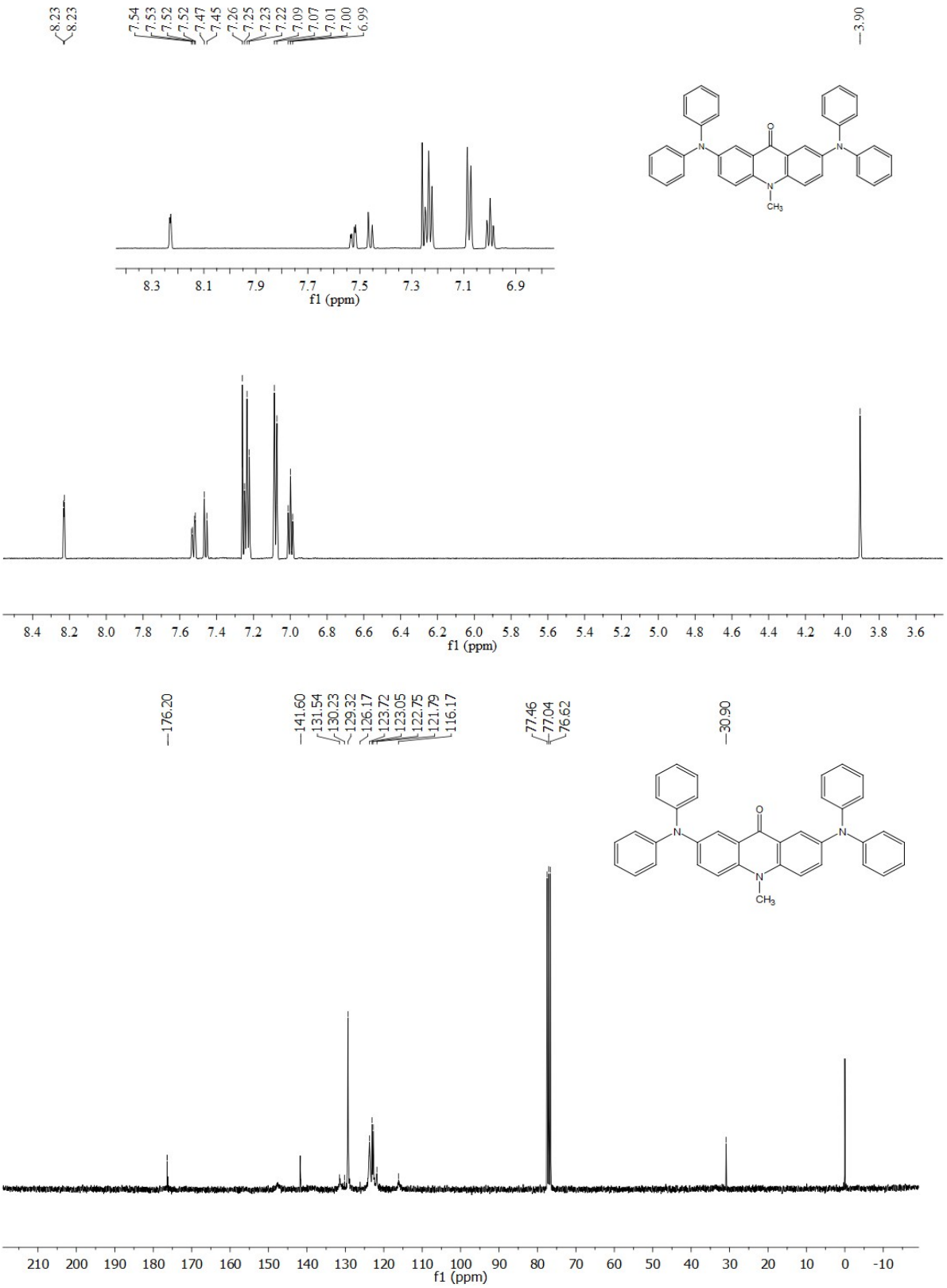
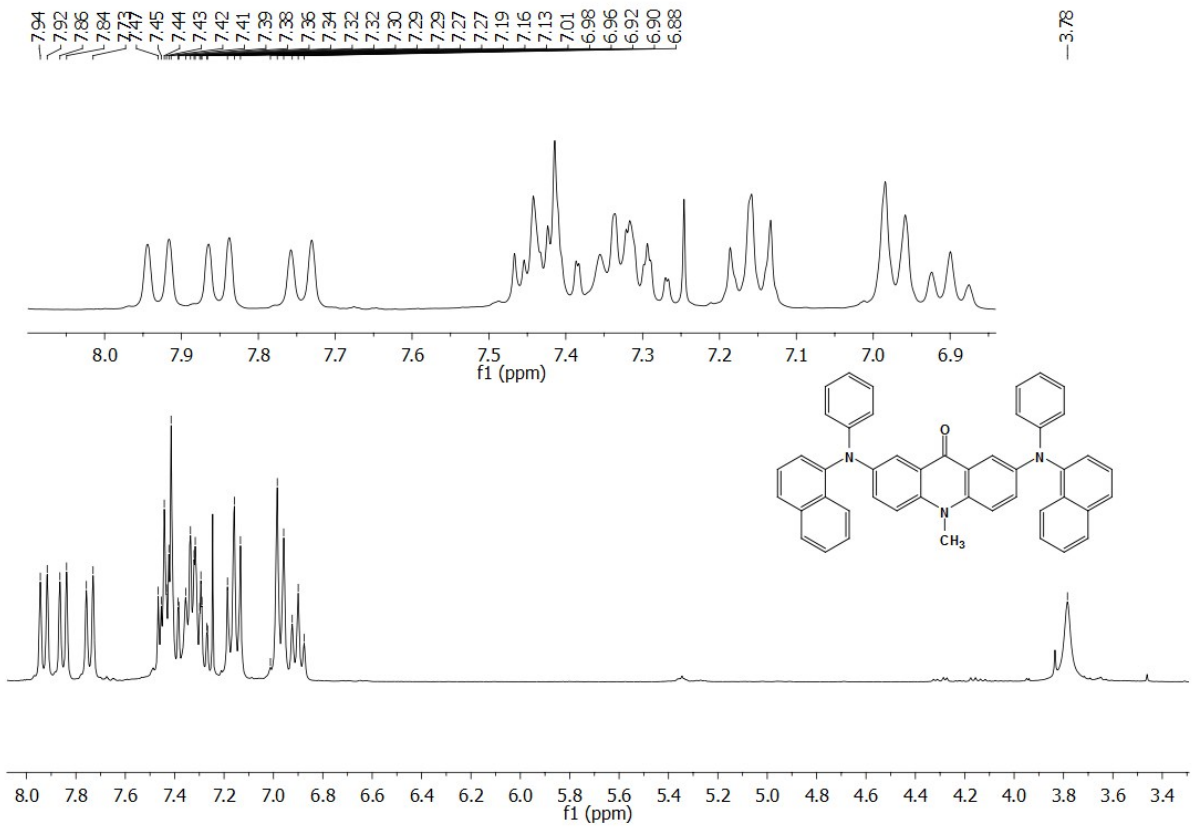


Figure S1: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra of **1** in $CDCl_3$.



[1]H NMR Spectra of compounds **2**

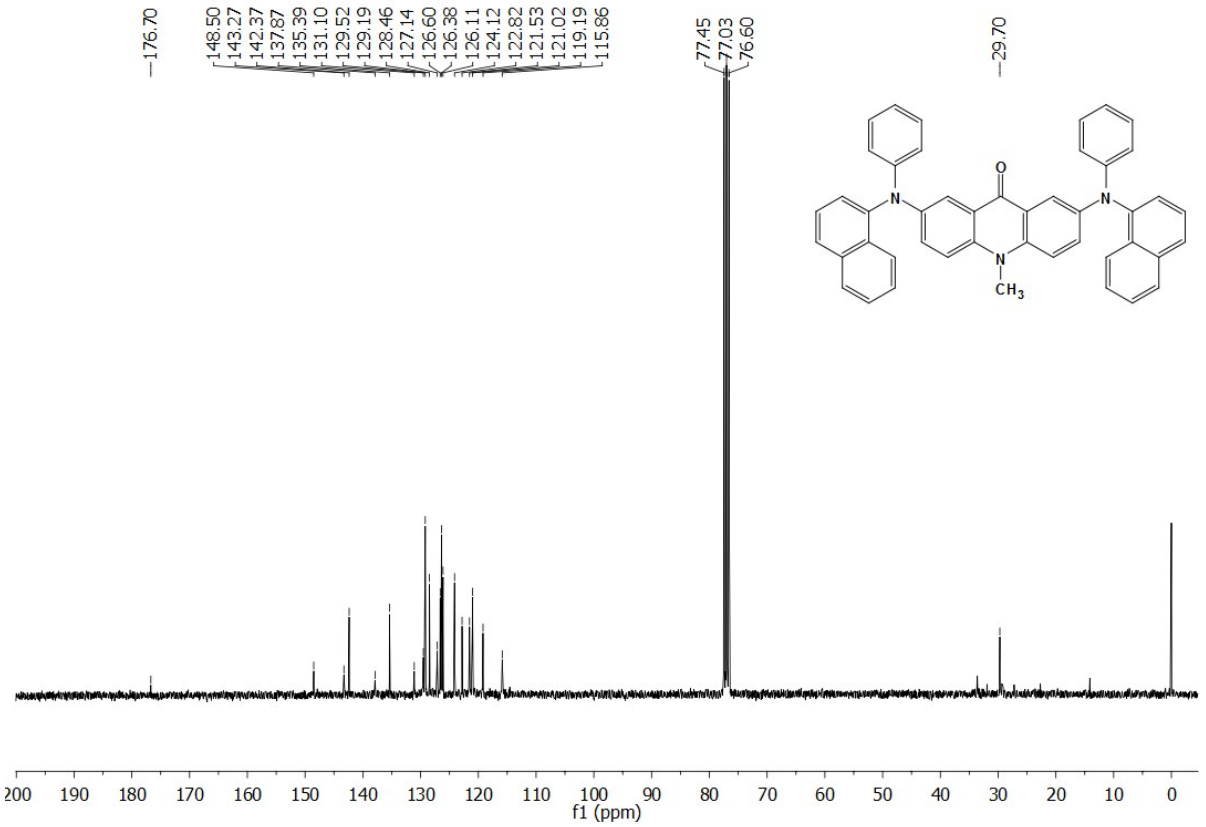
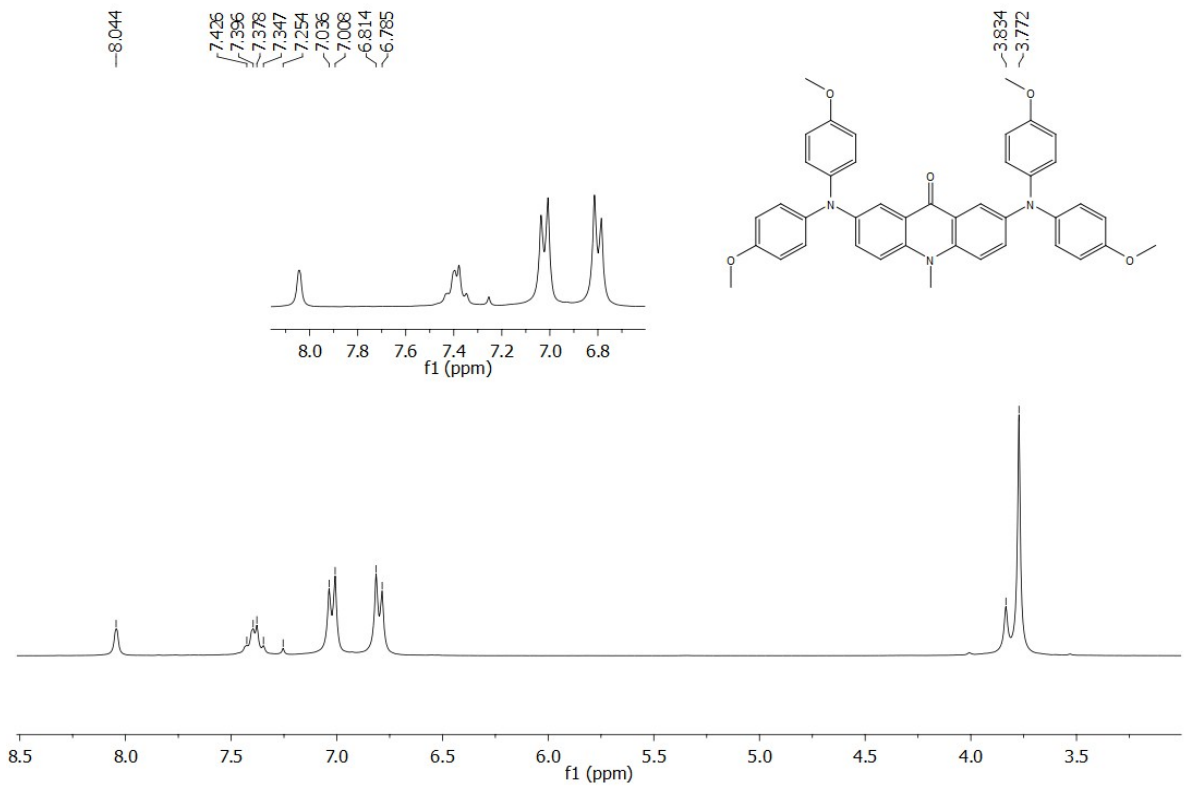


Figure S2: [1]H-NMR (above) and [13]C-NMR (below) spectra of **2** in $CDCl_3$.



I

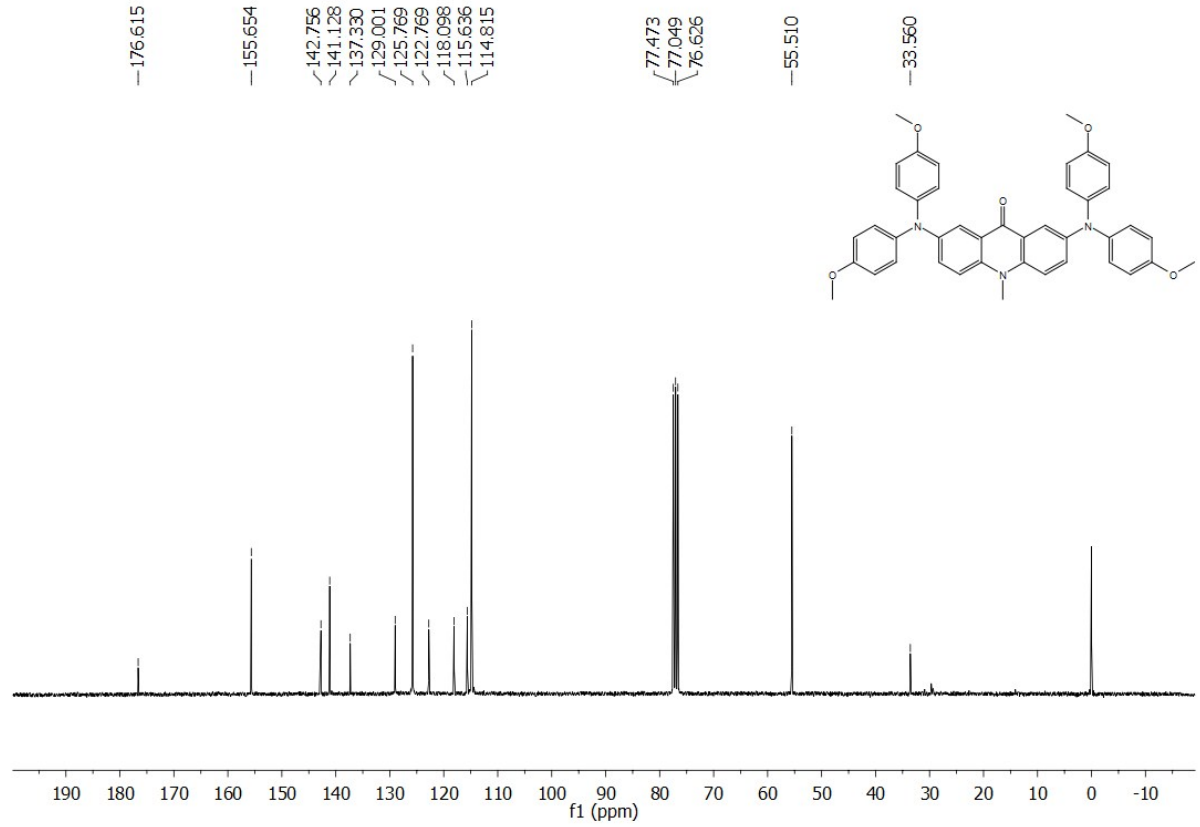


Figure S3: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra of **3** in $CDCl_3$.

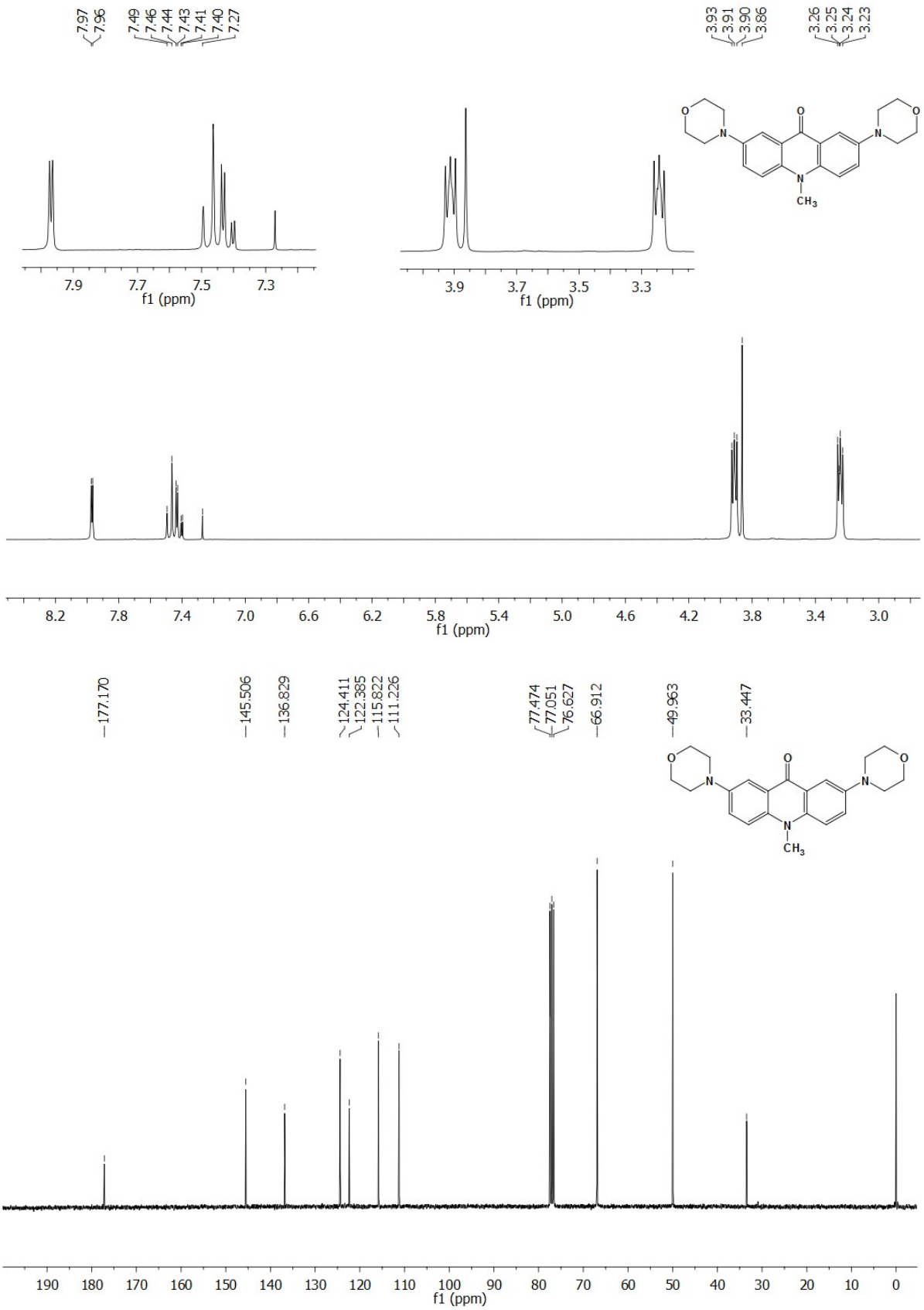


Figure S4: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra of **5** in $CDCl_3$.

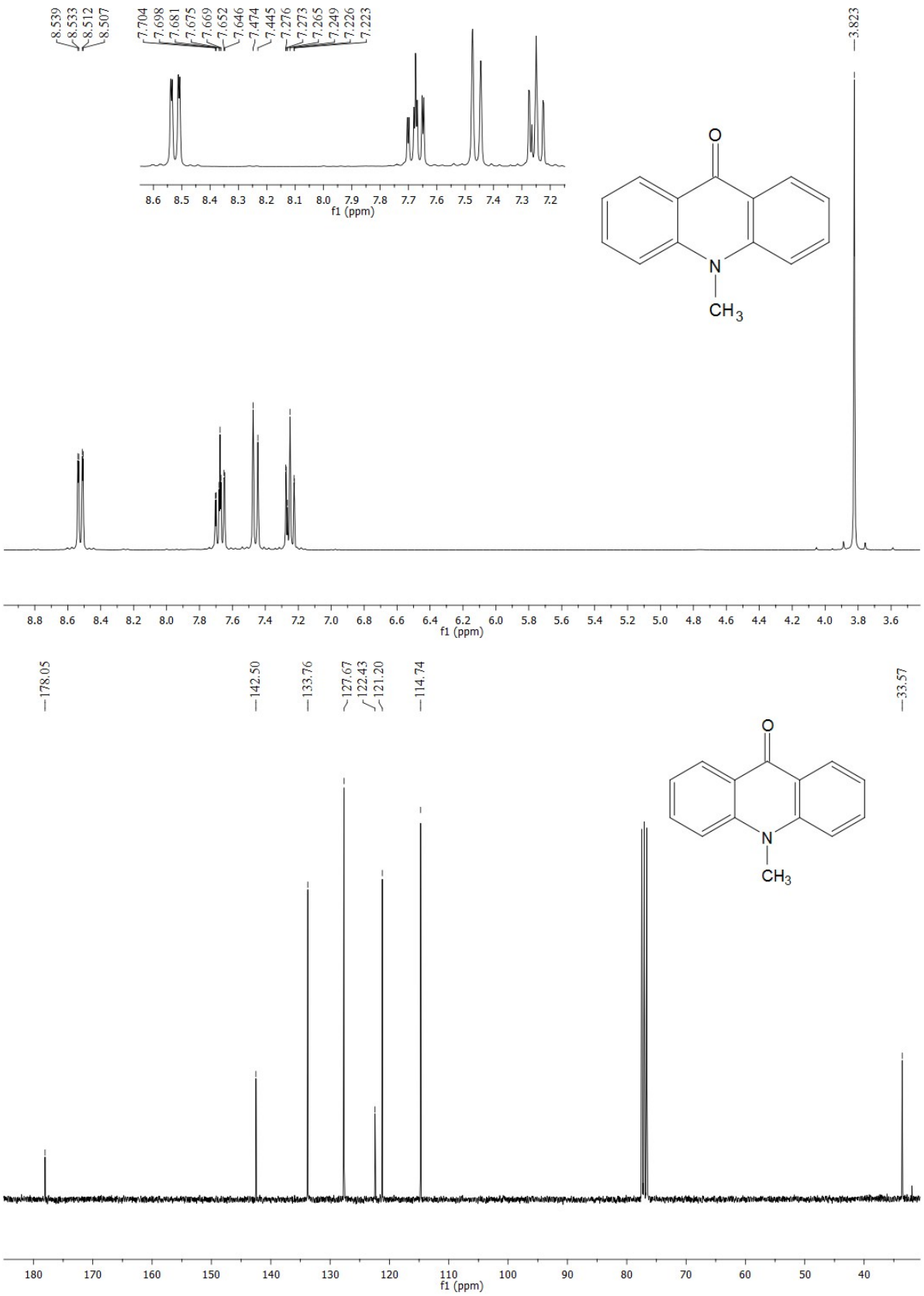


Figure S5: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra of **6** in $CDCl_3$.

Figure S6: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra of **7** in $CDCl_3$.

2) MALDI-TOF mass of compound 1-5:

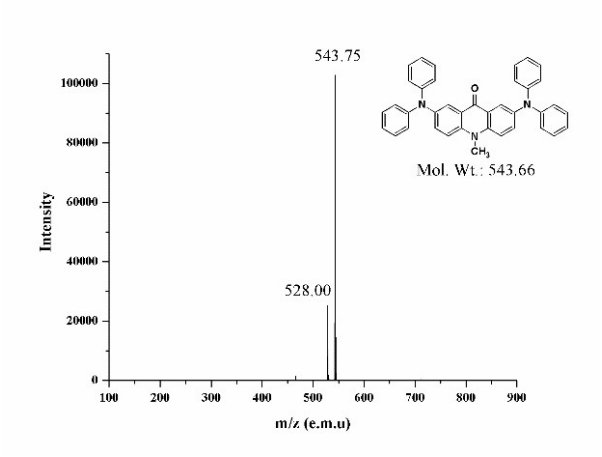


Figure S7: MALDI-TOF mass of **1**

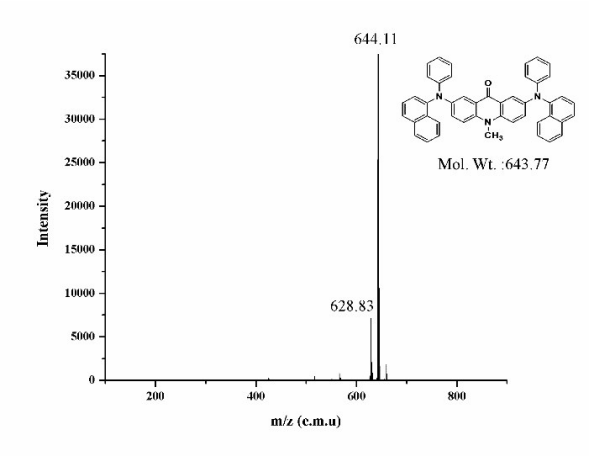


Figure S8: MALDI-TOF mass of **2**

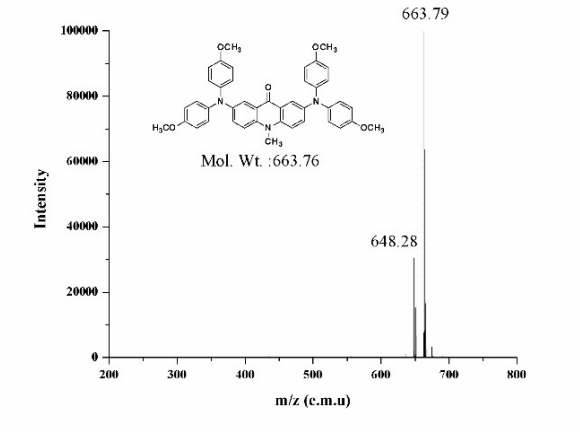


Figure S9: MALDI-TOF mass of **3**

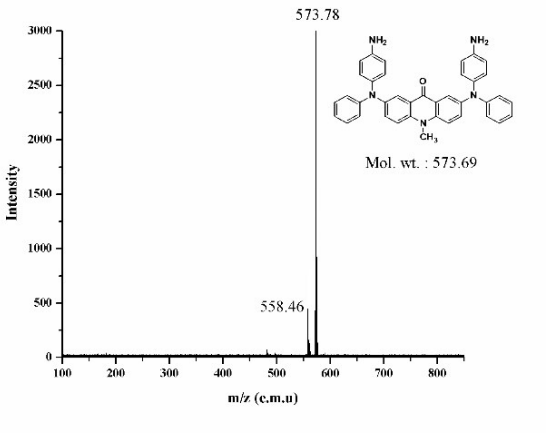


Figure S10: MALDI-TOF mass of **4**

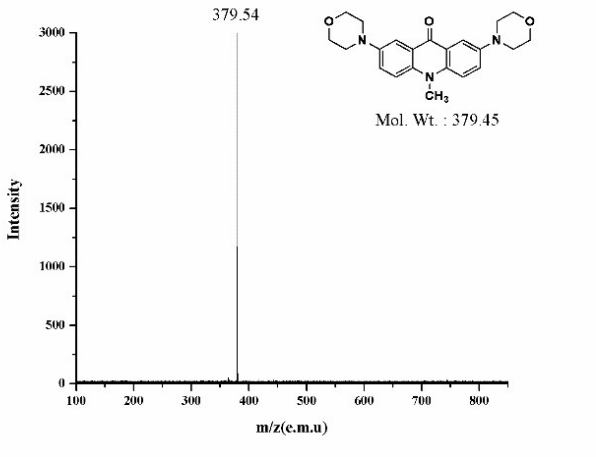


Figure S11: MALDI-TOF mass of **5**

3) **FT-IR Spectra of compound 1-5**

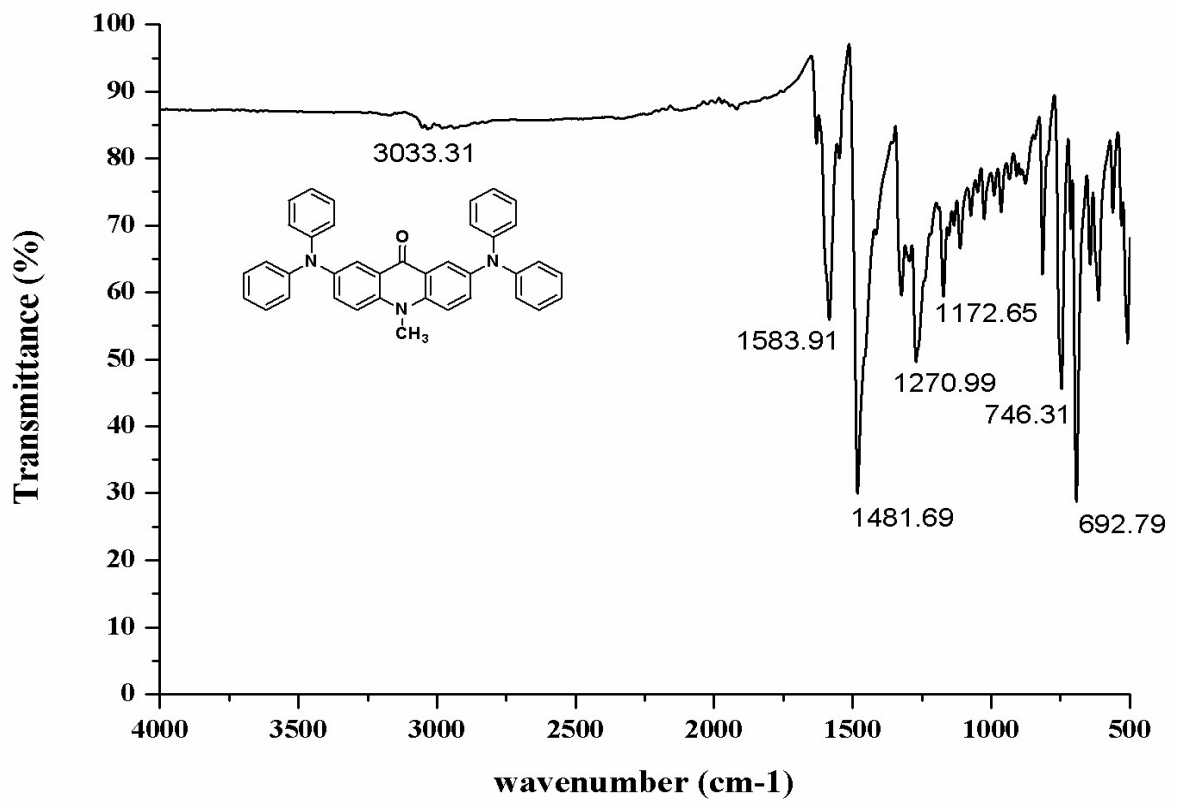


Figure S12: FTIR Spectra of **1.**

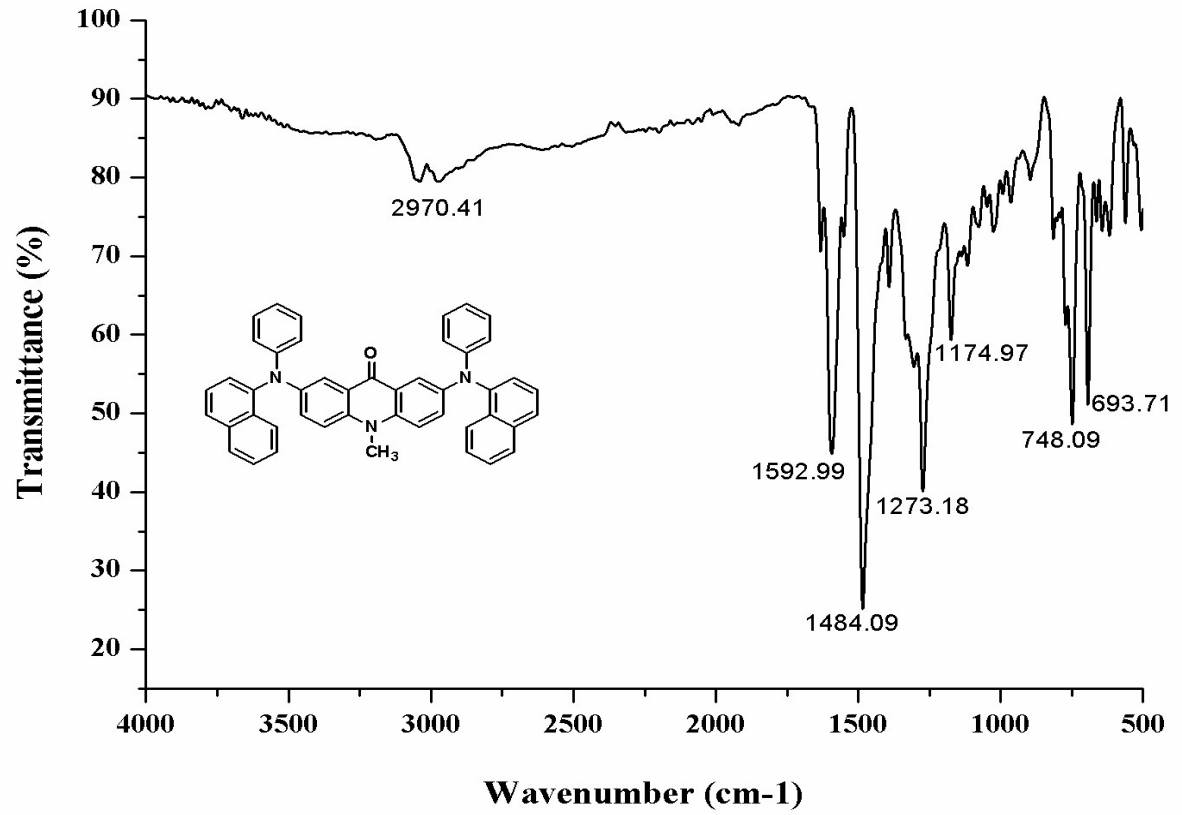


Figure S13: FTIR Spectra of **2.**

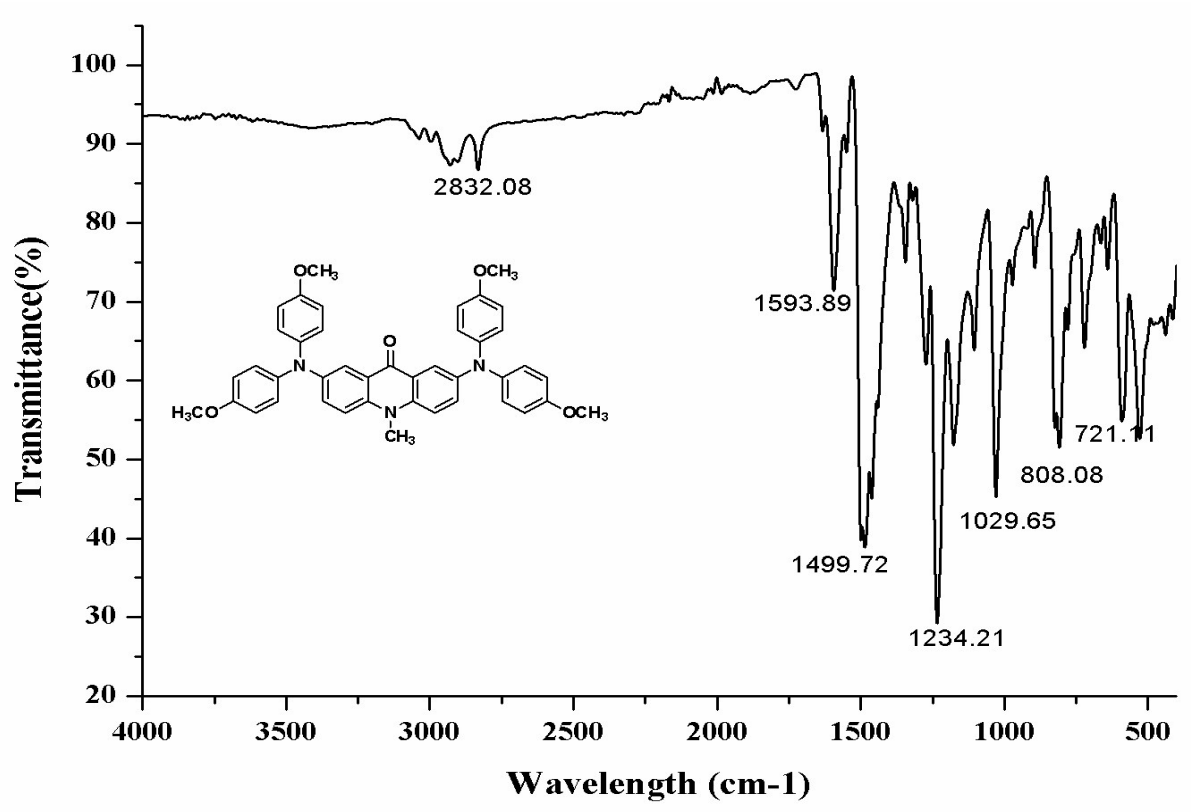


Figure S14: FTIR Spectra of **3.**

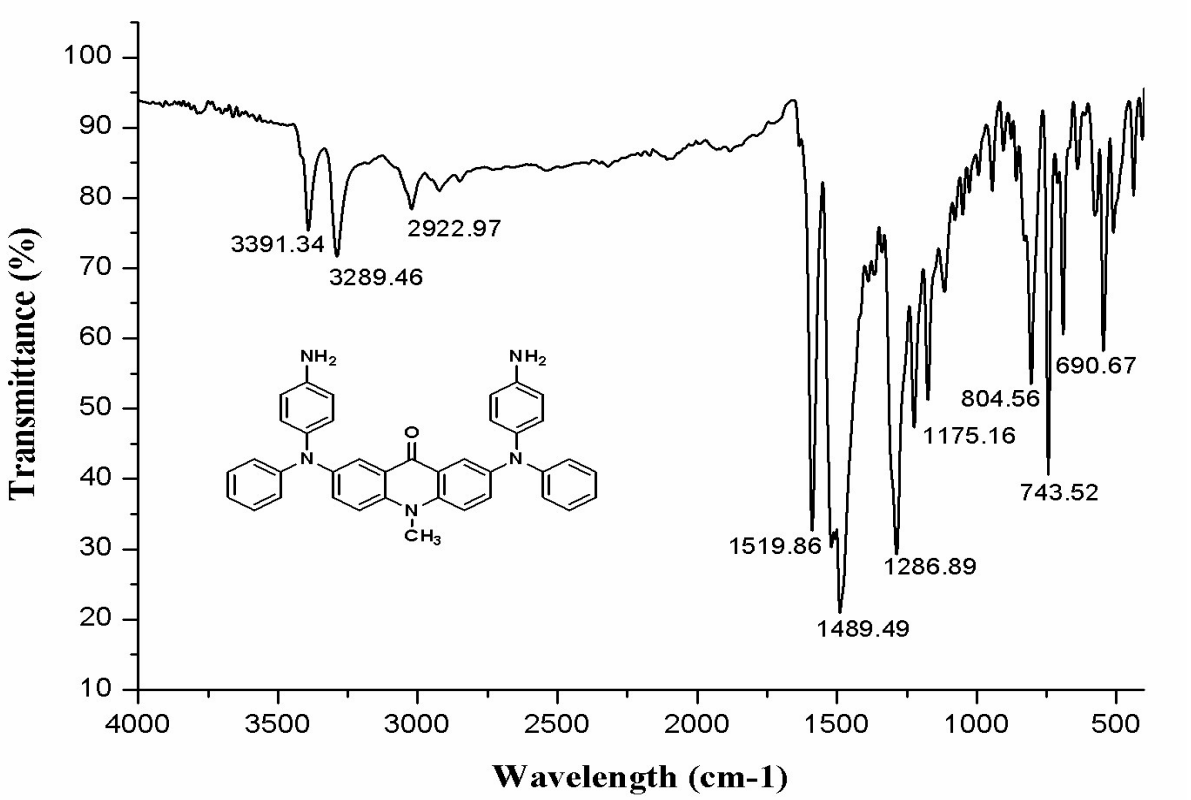


Figure S15: FTIR Spectra of **4.**

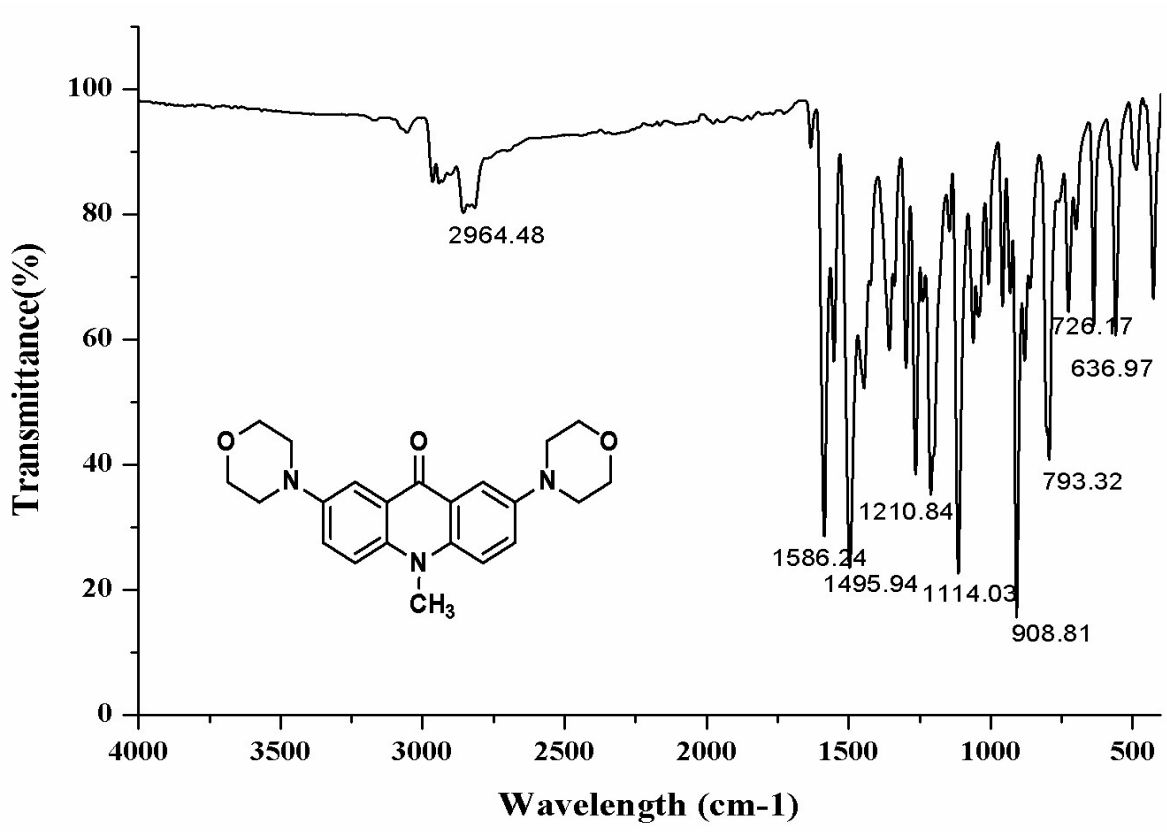


Figure S16: FTIR Spectra of **5.**

4) Photophysical data of compound 1-5 in various solvents:

i) Photophysical data of **1** in various solvents:

Solvent	**λ_{abs}[a], nm**	**λ_{em}[c], nm**	**Stokes shift [d], cm^{-1}**	**E_g^{opt} eV**
Toluene	303, 348, 397, 458	501	1873.98	2.55
Dichloromethane	303, 348, 401, 462	522	2487.93	2.51
Ethyl acetate	299, 344, 392, 451	504	2331.67	2.62
Acetonitrile	305, 344, 396, 458	520	2603.29	2.53
Dimethylsulphoxide	301, 349, 400, 463	523	2477.81	2.54

ii) Photophysical data of **2** in various solvents:

Solvent	**λ_{abs}[a], nm**	**λ_{em}[c], nm**	**Stokes shift [d], cm^{-1}**	E_g^{opt} **eV**
Toluene	338, 360, 459	500	1786.49	2.55
Dichloromethane	339, 359, 461	519	2424.15	2.54
Ethyl acetate	335, 355, 443	501	2613.28	2.67
Acetonitrile	336, 351, 450	517	2879.86	2.56
Dimethylsulphoxide	340, 359, 455	518	2673.00	2.56

iii) Photophysical data of **3** in various solvents:

Solvent	**λ_{abs}[a], nm**	**λ_{em}[c], nm**	**Stokes shift [d], cm^{-1}**	E_g^{opt} **eV**
Toluene	303, 353, 415, 478	528	1981.10	2.44
Dichloromethane	301, 351, 416, 483	558	2782.78	2.30
Ethyl acetate	299, 348, 406, 470	527	2301.26	2.50
Acetonitrile	301, 346, 412, 478	558	2999.35	2.46
Dimethylsulphoxide	301, 351, 416, 483	540	2185.41	2.53

iv) Photophysical data of **4** in various solvents:

Solvent	**λ_{abs}[a], nm**	**λ_{em}[c], nm**	**Stokes shift [d], cm^{-1}**	E_g^{opt} **eV**
Toluene	310, 338, 460	519	2471.30	2.55
Dichloromethane	312, 339, 392, 464	522	2394.63	2.63
Ethyl acetate	313, 340, 390, 463	517	2255.91	2.62
Acetonitrile	310, 339, 393, 462	522	2487.93	2.66
Dimethylsulphoxide	318, 351, 408, 488	527	1516.47	2.62

v) Photophysical data of **5** in various solvents:

Solvent	**λ_{abs}[a], nm**	**λ_{em}[c], nm**	**Stokes shift [d], cm^{-1}**	E_g^{opt} **eV**
Toluene	309, 362, 446	512	2890.27	2.66
Dichloromethane	308, 360, 448	523	3200.00	2.56
Ethyl acetate	305, 355, 439	513	3285.86	2.63
Acetonitrile	307, 360, 445	525	3424.29	2.57
Dimethylsulphoxide	311, 364, 450	529	3318.63	2.55

5) Absorption and Emission spectra of compound 1-5 in various solvents:-

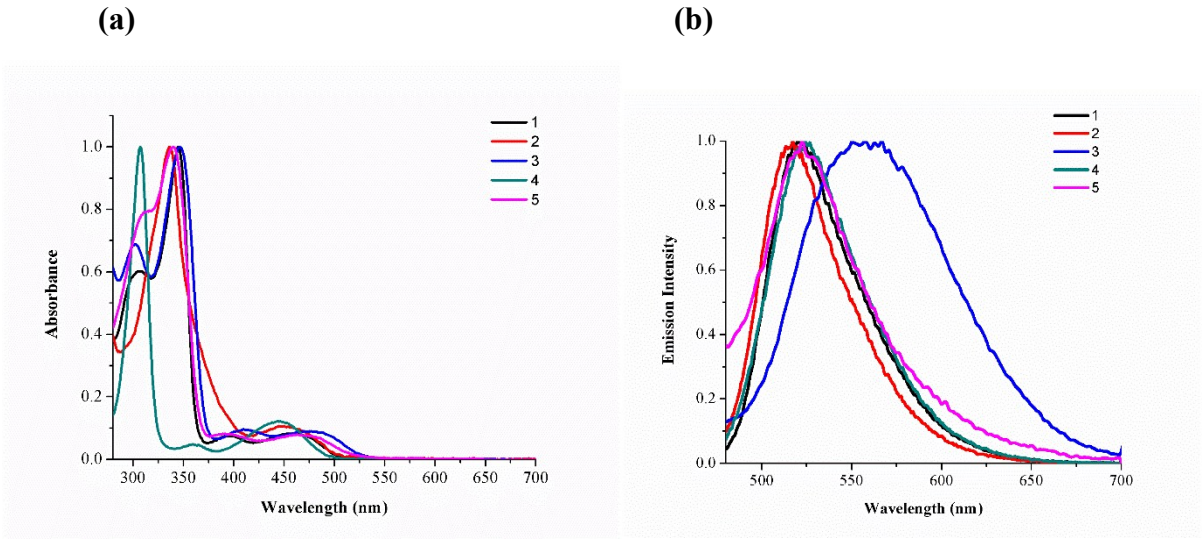


Figure S17: Absorption spectra (a) and Emission spectra (b) of 1-5 in **dichloromethane.**

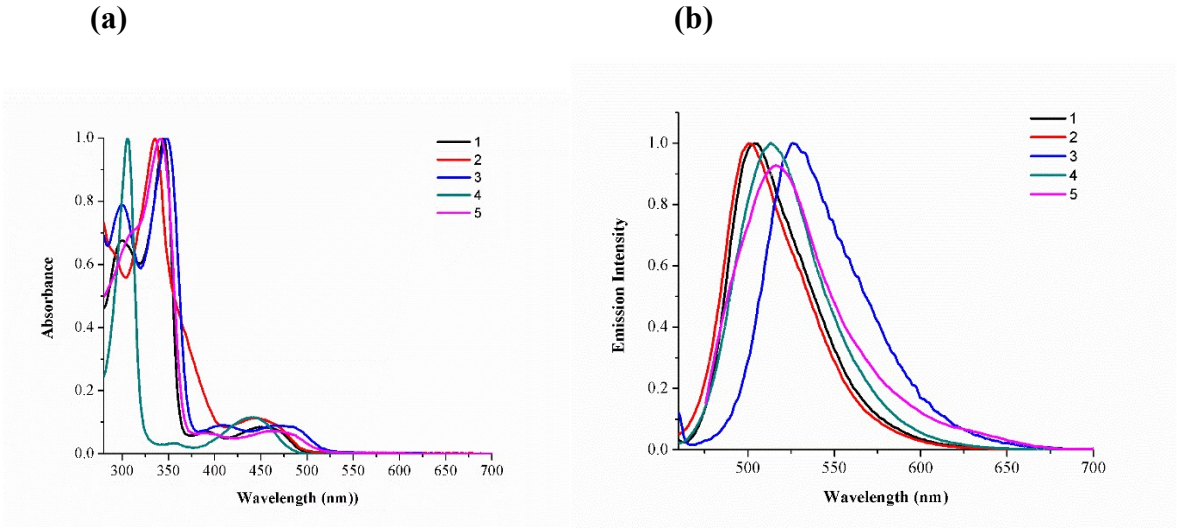


Figure S18: Absorption spectra (a) and Emission spectra (b) of 1-5 in **ethyl acteate.**

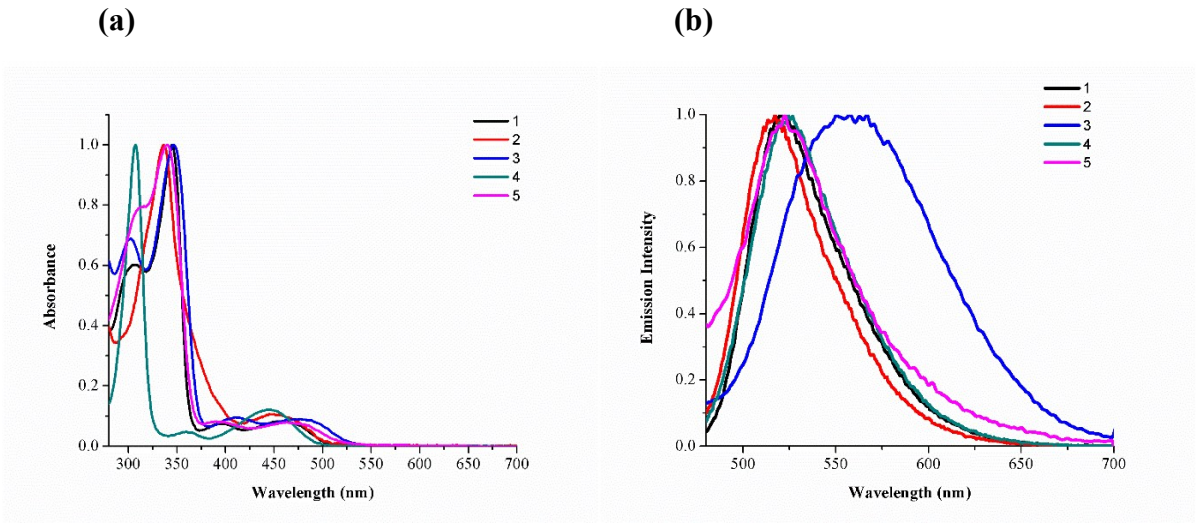


Figure S19: Absorption spectra (a) and Emission spectra (b) of 1-5 in **Acetonitrile.**

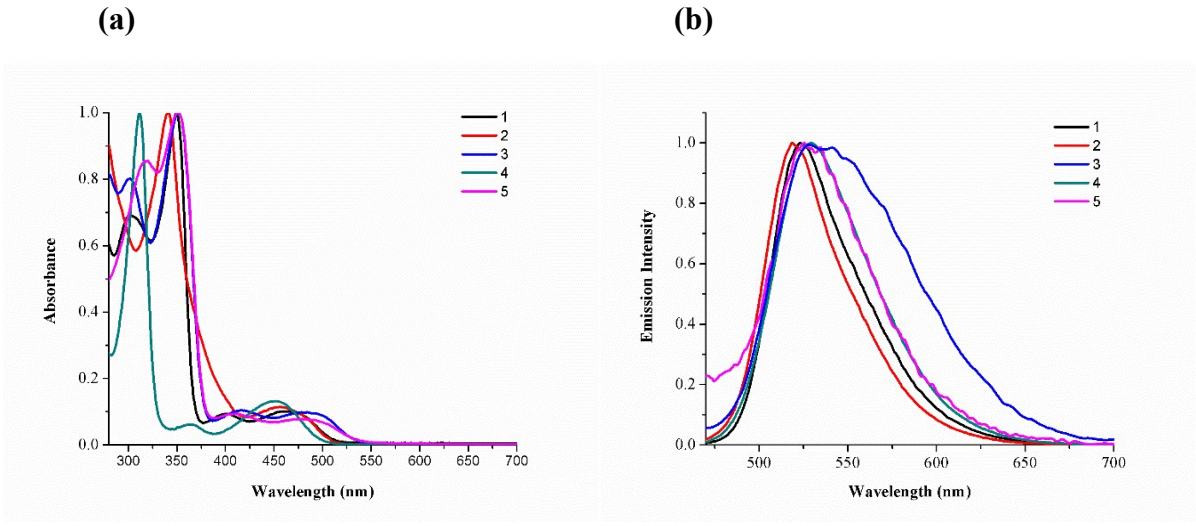


Figure S20: Absorption spectra (a) and Emission spectra (b) of 1-5 in **dimethylsulphoxide**

6) Life time measurement spectra of compounds 1-5 in toluene:

Table 2: Life time data of **1-5** in toluene

Compound	Wavelength (nm)	τ_1 ns (a_1)	τ_2 ns (a_2)
1	475	1.16 (0.86)	11.83 (0.14)
	501	1.20 (0.23)	13.44 (0.77)
	580	1.05 (0.05)	13.75 (0.95)
2	480	1.14 (0.23)	11.29 (0.77)
	500	1.34 (0.07)	12.2 (0.93)
	560	12.32	----
3	490	1.16 (0.84)	10.72 (0.16)
	527	1.49 (0.11)	12.56 (0.89)
	560	1.51 (0.03)	12.63 (0.97)
4	490	1.1 (0.86)	5 (0.14)
	518	1.49 (0.8)	5 (0.2)
	560	1.94 (0.88)	8.31 (0.12)
5	490	1.15 (0.74)	11.3 (0.26)
	512	1.18 (0.37)	12.22 (0.63)
	560	1.11 (0.15)	12.28 (0.85)

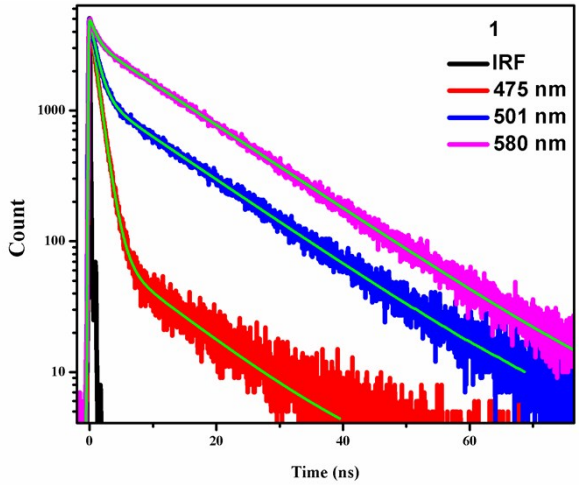


Figure S21: Life time spectra of **1.**

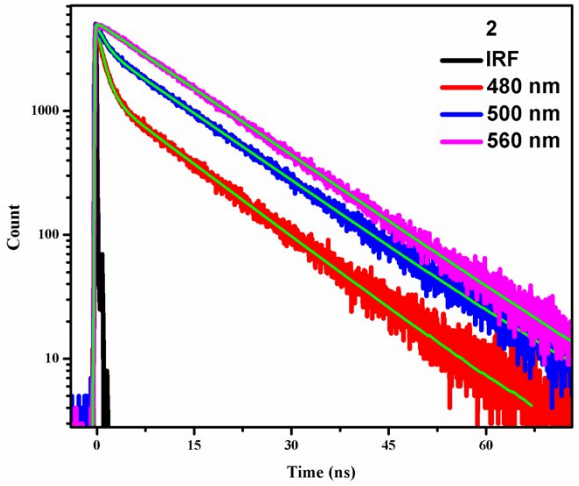


Figure S22: Life time spectra of **2.**

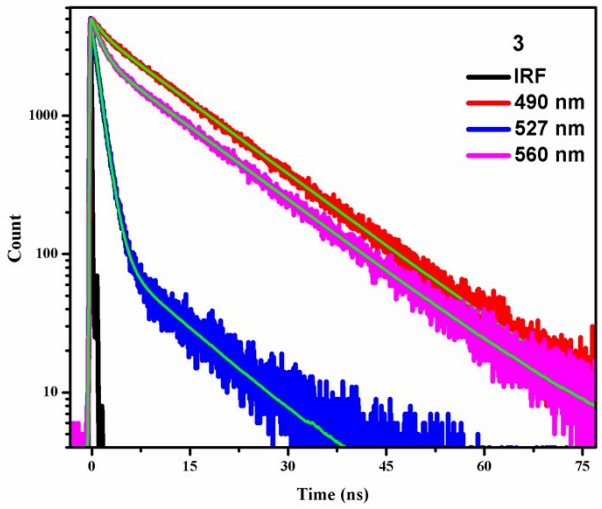


Figure S23: Life time spectra of **3.**

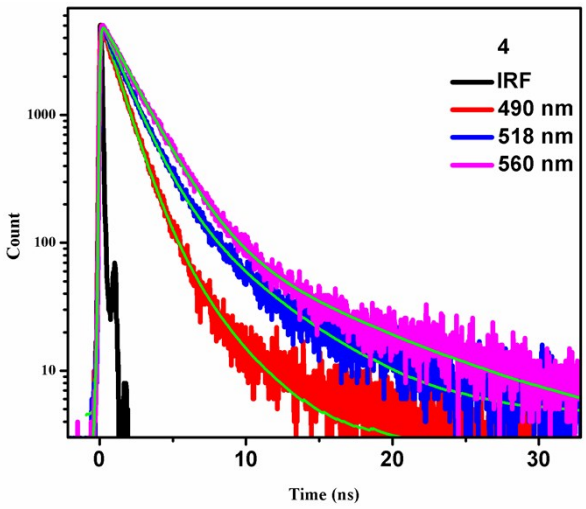


Figure S24: Life time spectra of **4**

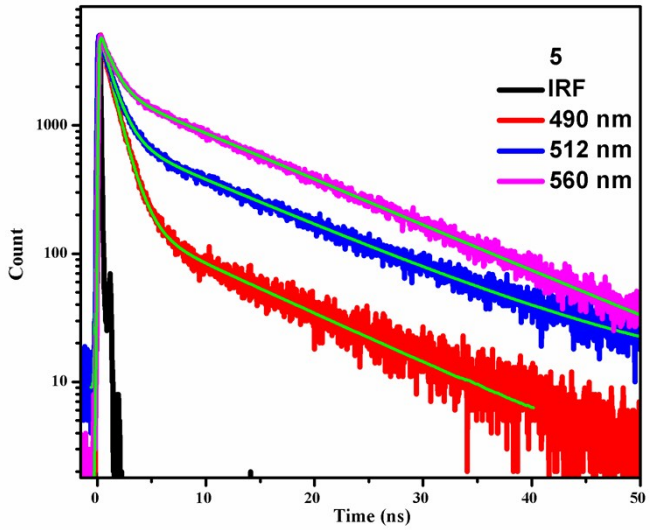


Figure S25: Life time spectra of **5.**

7) Cyclic voltammetry and differential pulse voltammetry of compounds 1-5 in acetonitrile :-

(a) **(b)**

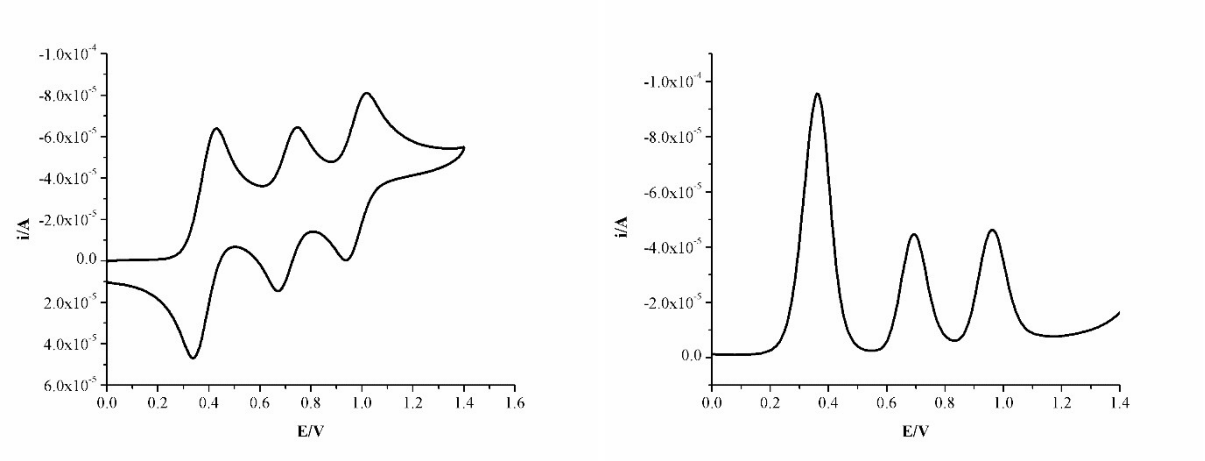


Figure S26: Cyclic voltammetry (a) and differential pulse voltammetry (b) of **1**

(a) **(b)**

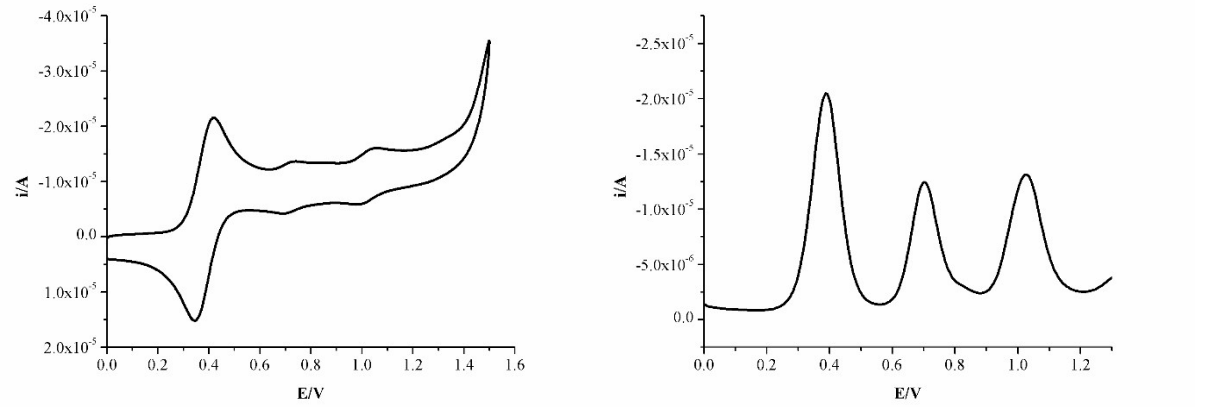


Figure S27: Cyclic voltammetry (a) and differential pulse voltammetry (b) of **2**

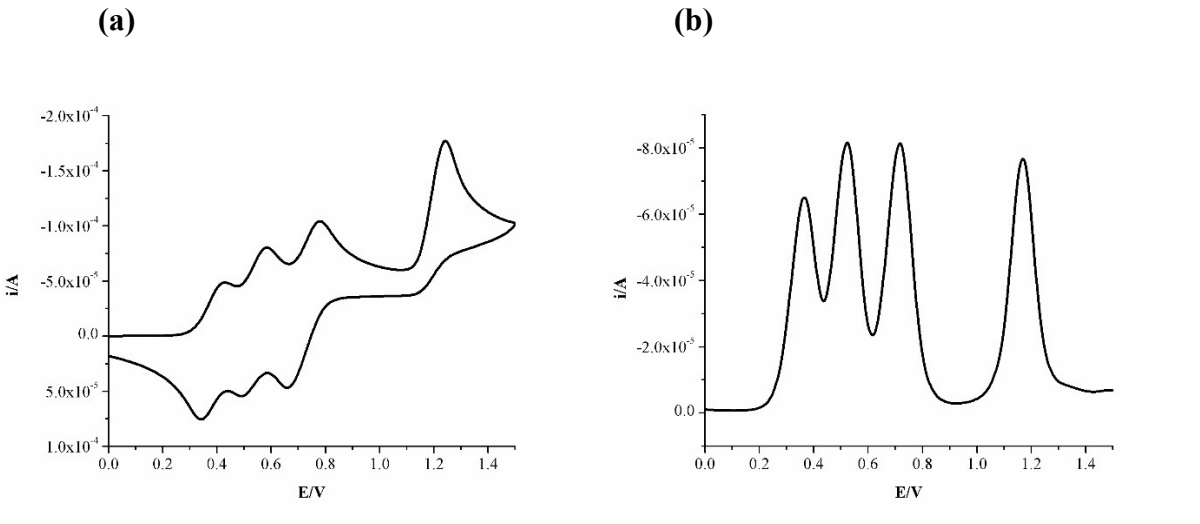


Figure S28: Cyclic voltammetry (a) and differential pulse voltammetry (b) of **3**

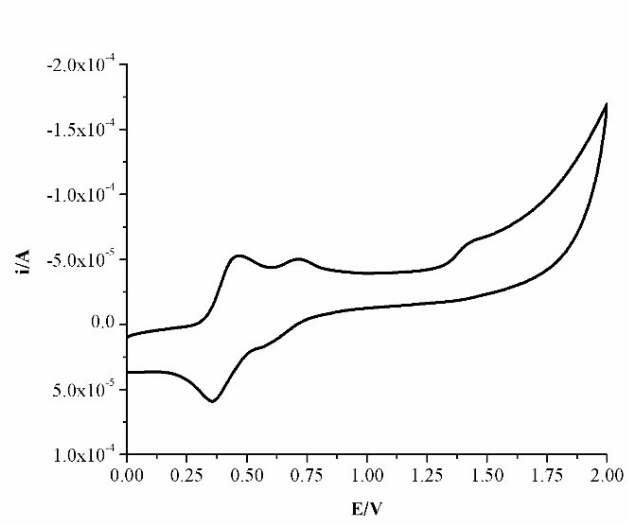


Figure S29: Cyclic voltammetry of **4:**

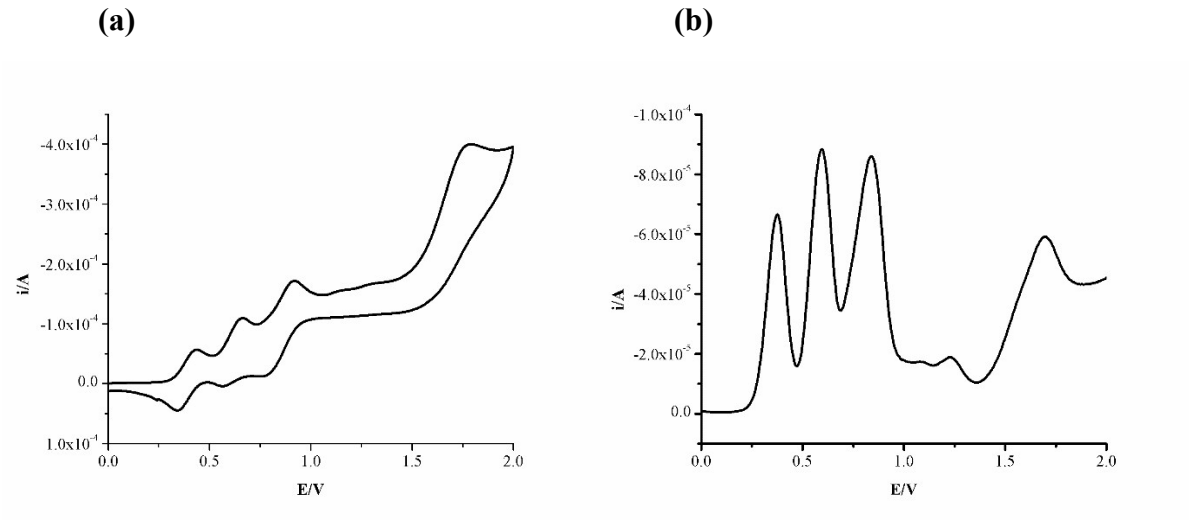


Figure S30: Cyclic voltammetry (a) and differential pulse voltammetry (b) of **5:**

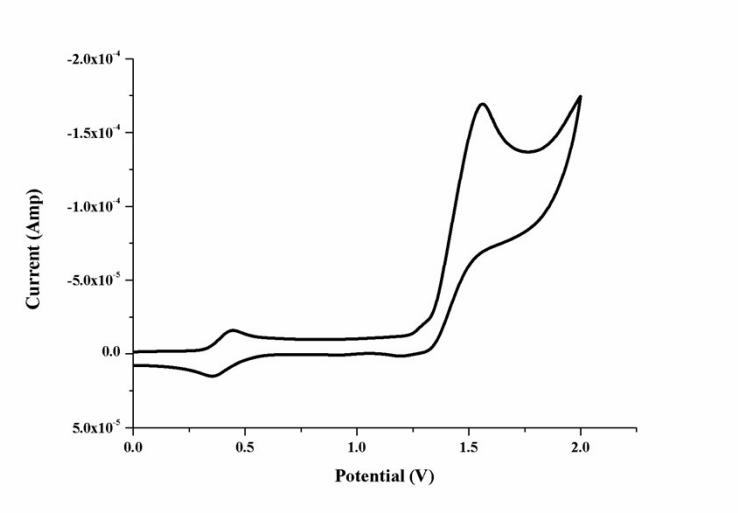


Figure S31: Cyclic voltammetry of **6** (9-methylacridone):

8) Thermo-Gravimetric (TG) and Differential thermogravimetric (DTG) plots of compounds 1-5 :-

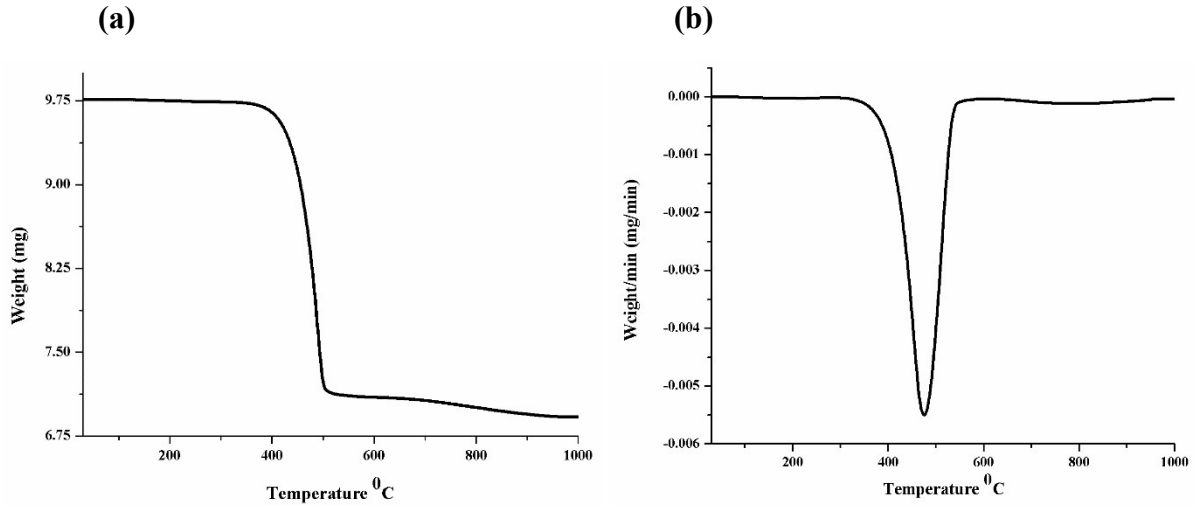


Figure S32: TG (a) and DTG (b) plots of **1**

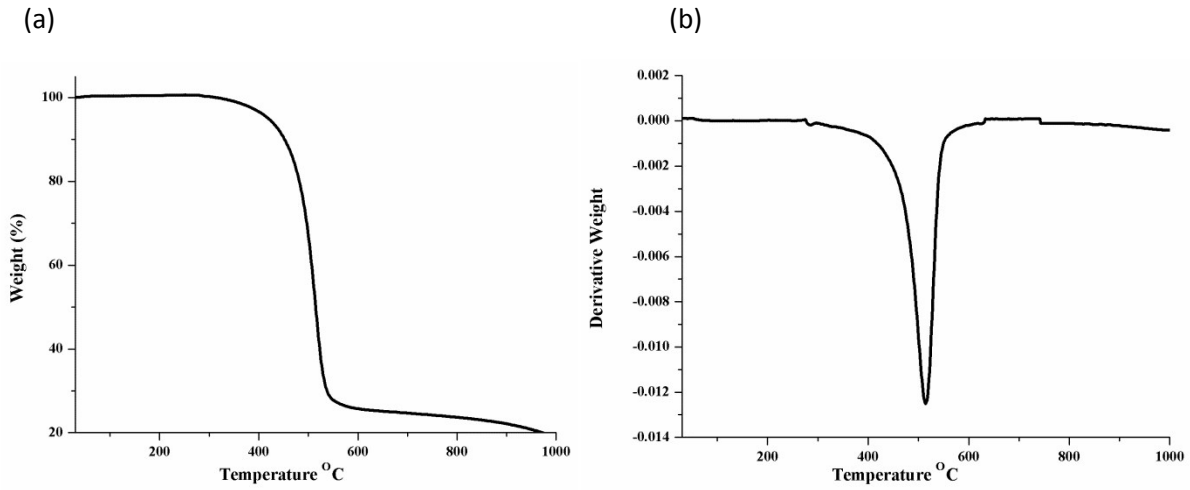


Figure S33: TG (a) and Derivative weight loss (b) plots of **2**.

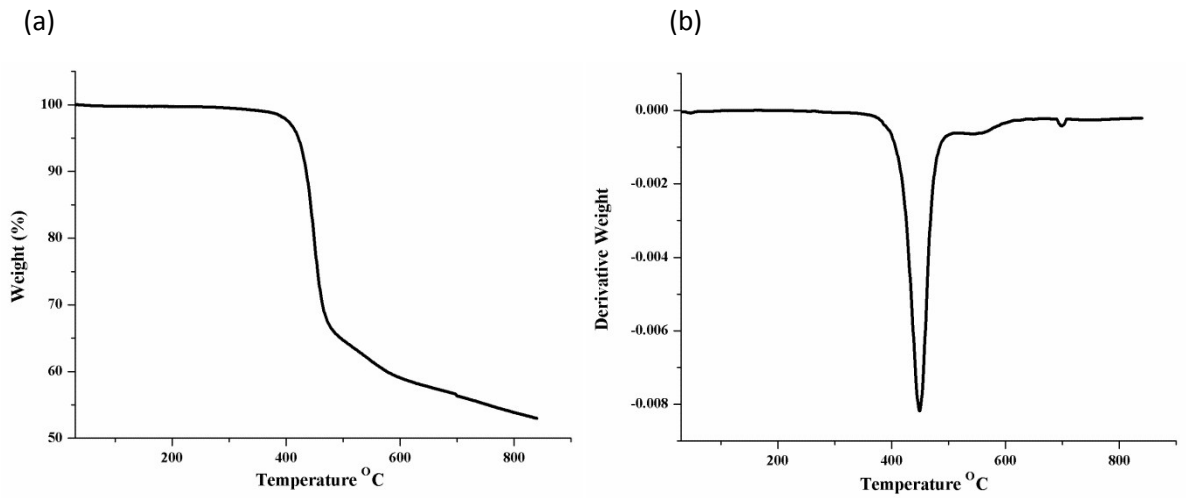


Figure S34: TG (a) and Derivative weight loss (b) plots of **3**.

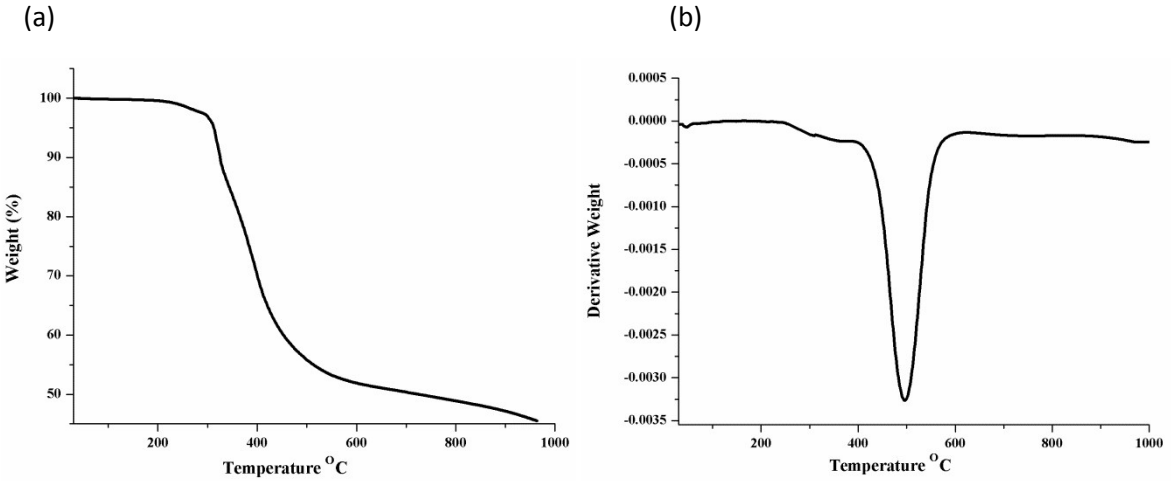


Figure S35: TG (a) and Derivative weight loss (b) plots of **4**.

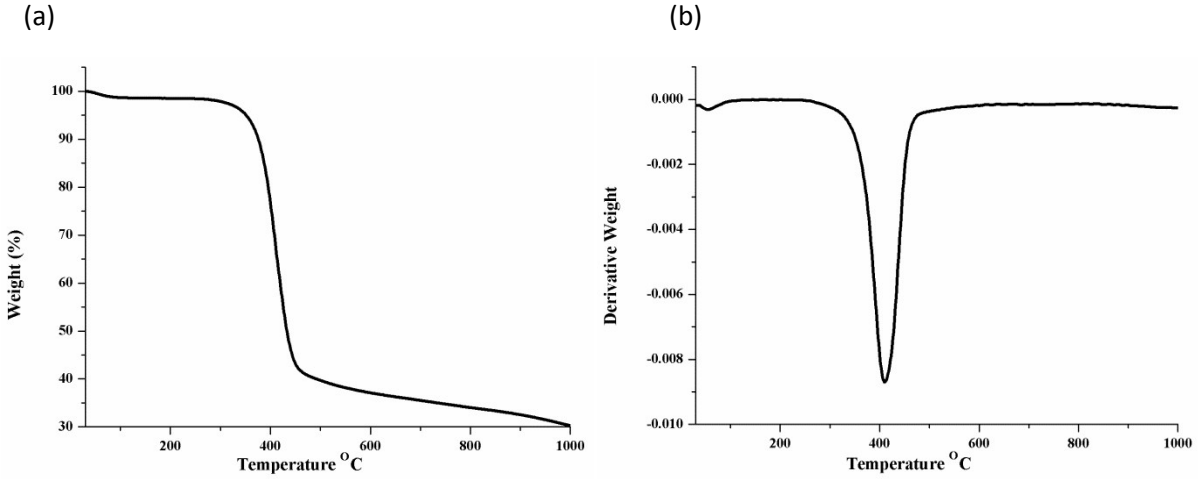


Figure S36: TG (a) and Derivative weight loss (b) plots of **5**.