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

Supporting Information

Phenanthroimidazole derivatives showing mild intramolecular charge transfer, high quantum yield and their applications in OLEDs

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Contents:

Characterization and Spectroscopic data of 1

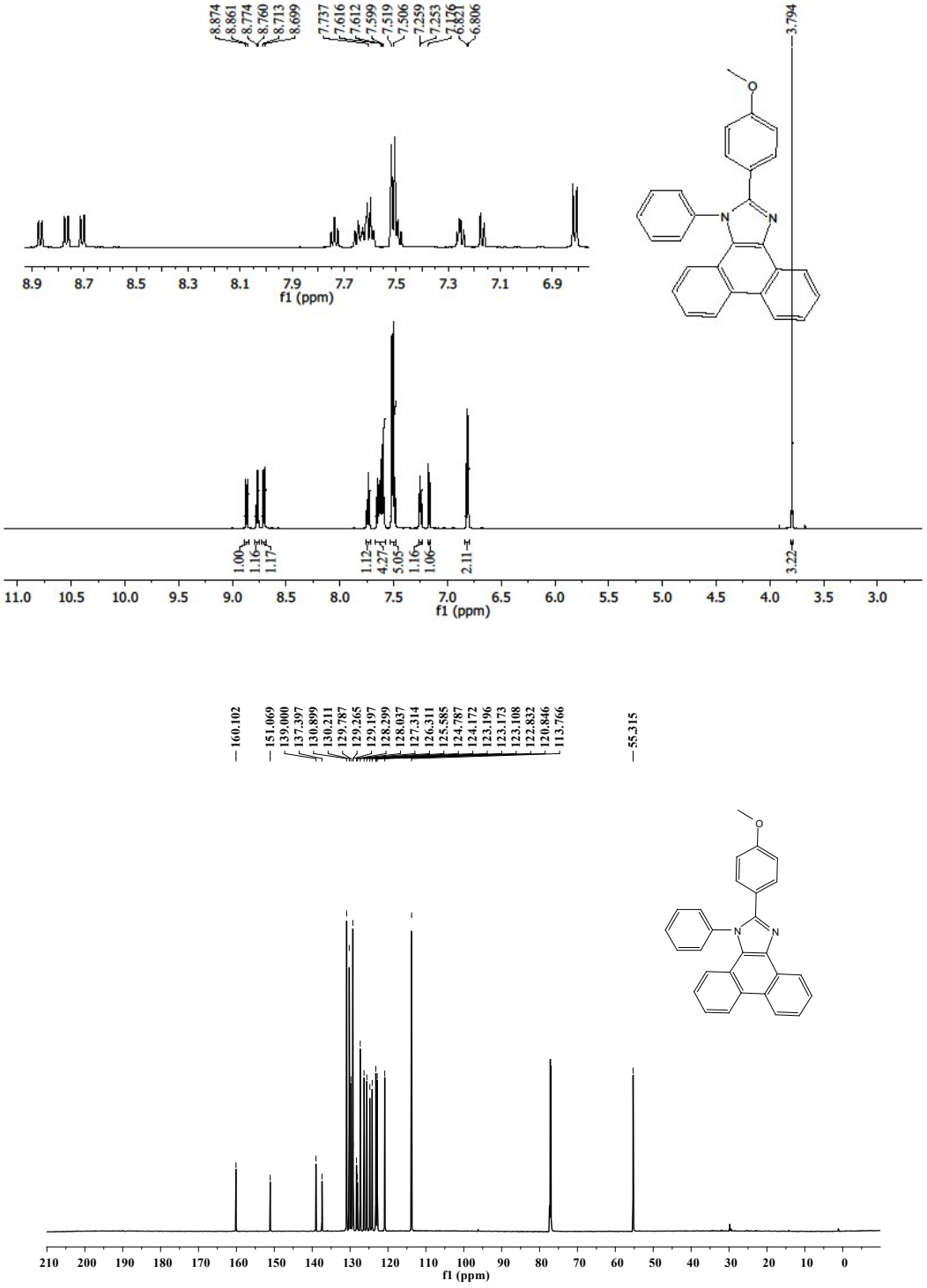

Figure SI 1: ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **1** in $CDCl_3$

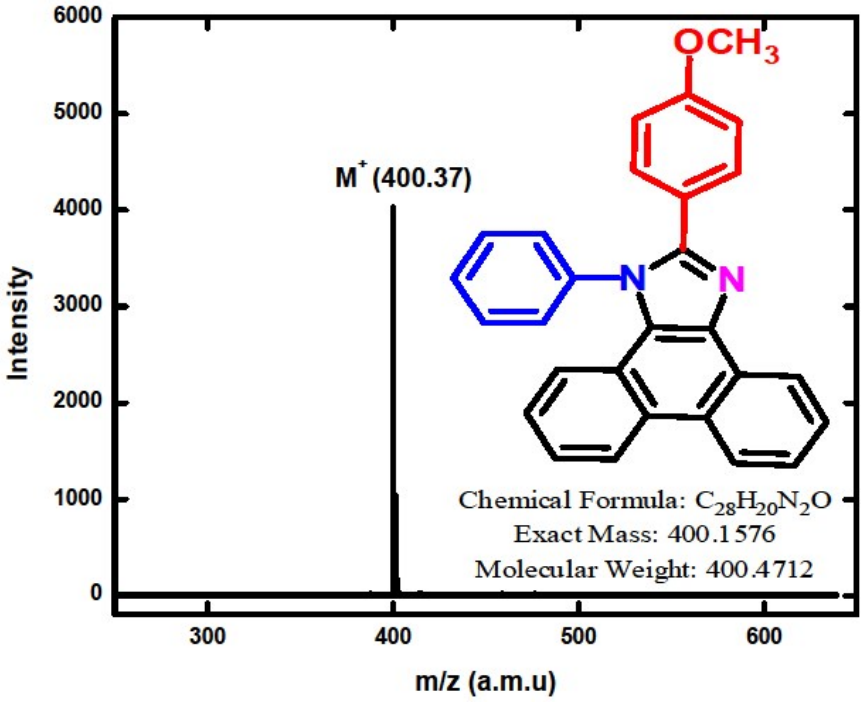

Figure SI 2: MALDI – TOF spectrum for **1**

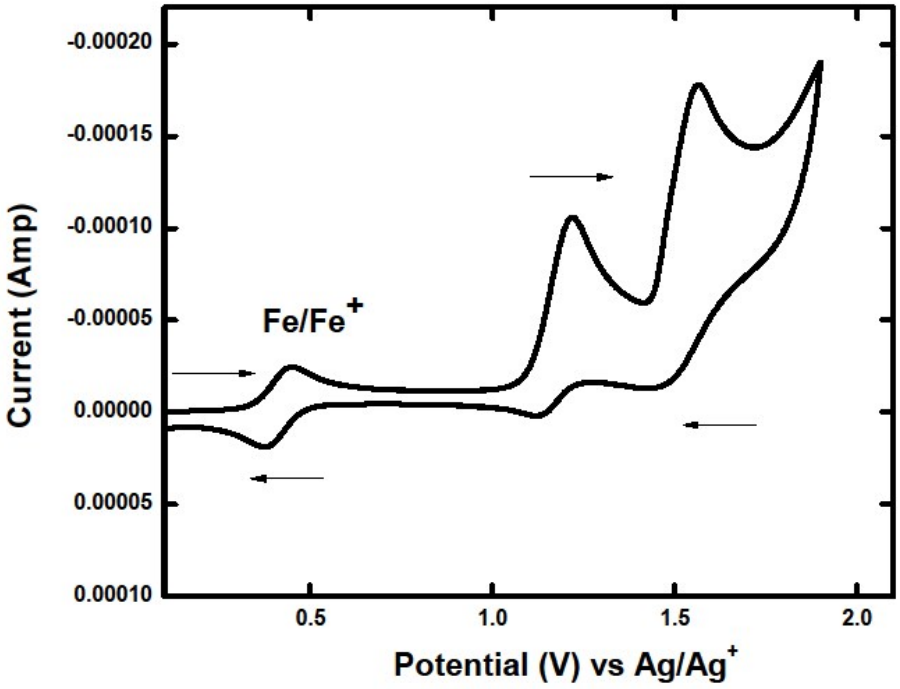

Figure SI 3: Cyclic voltammetry of **1.**

Photophysical studies:

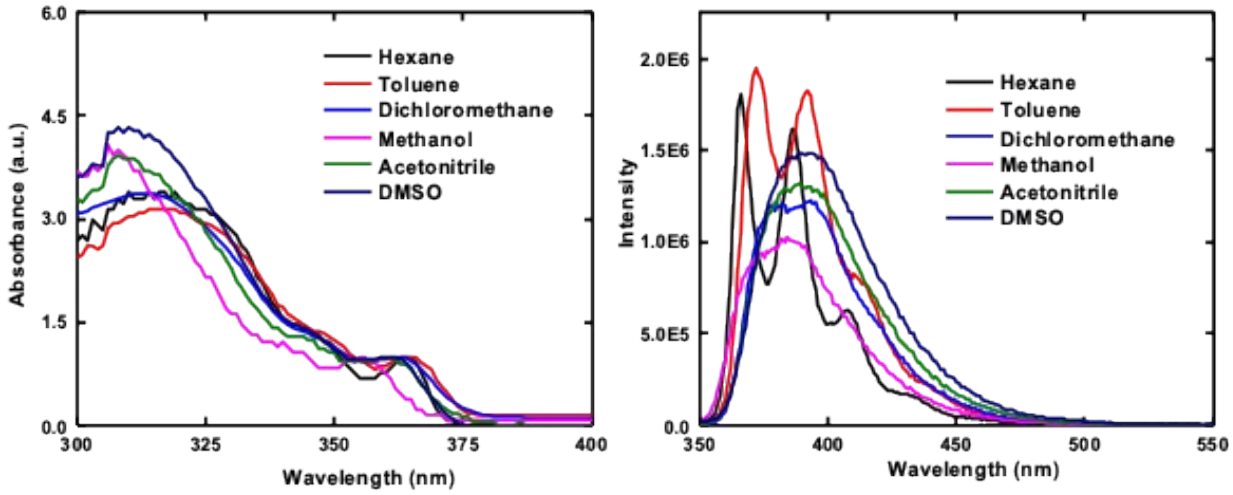

Figure SI 4: Absorption and emission spectra of **1** in different solvents

Table SI 1: Absorption and emission data of **1** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	364 (3.64), 345 (3.78), 316 (4.15), 261 (4.60)	366, 386, 407	1570	33	3.43
Toluene	364(3.84), 318(4.33), 288(4.35)	372,.391	1900	41	3.40
DCM	363(4.48), 315(4.98), 263(5.43)	377, 392	2030	38	3.43
CH_3OH	356(3.64), 308(4.23) 258(4.75)	381	1840	45	3.59
CH_3CN	361(3.73), 309(4.33), 260(4.89)	387	1870	40	3.43
DMSO	362(4.06), 310(4.63), 262(5.21)	391	2050	53	3.47

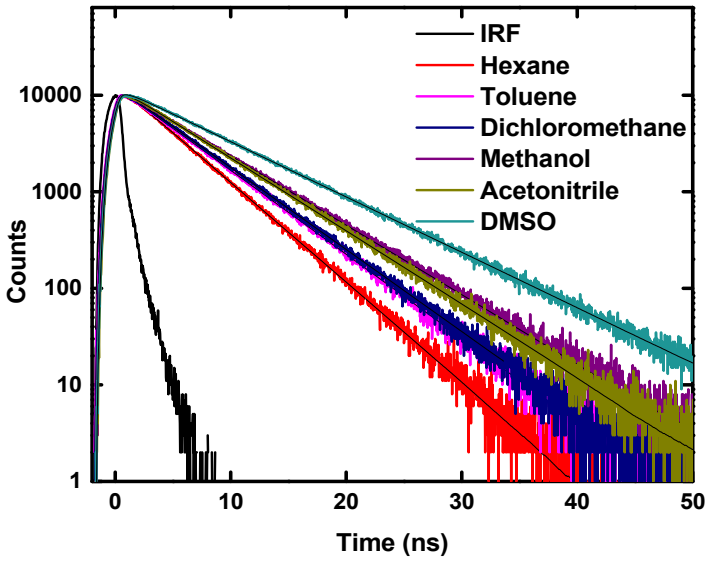

Figure SI 5: Fluorescence decay spectra of **1** in different solvents

Table SI 2: Fluorescence decay data of **1** in different solvents

Solvent	λ_{em}(nm)	τ_1(ns)	α	Chi sq
Hexane	407	4.21	100	1.00
Toluene	391	4.99.	100	1.15
DCM	392	5.11	100	1.20
CH_3OH	381	6.05	100	1.07
CH_3CN	387	5.76	100	1.00
DMSO	391	7.59	100	1.15

Characterization and Spectroscopic data of 2

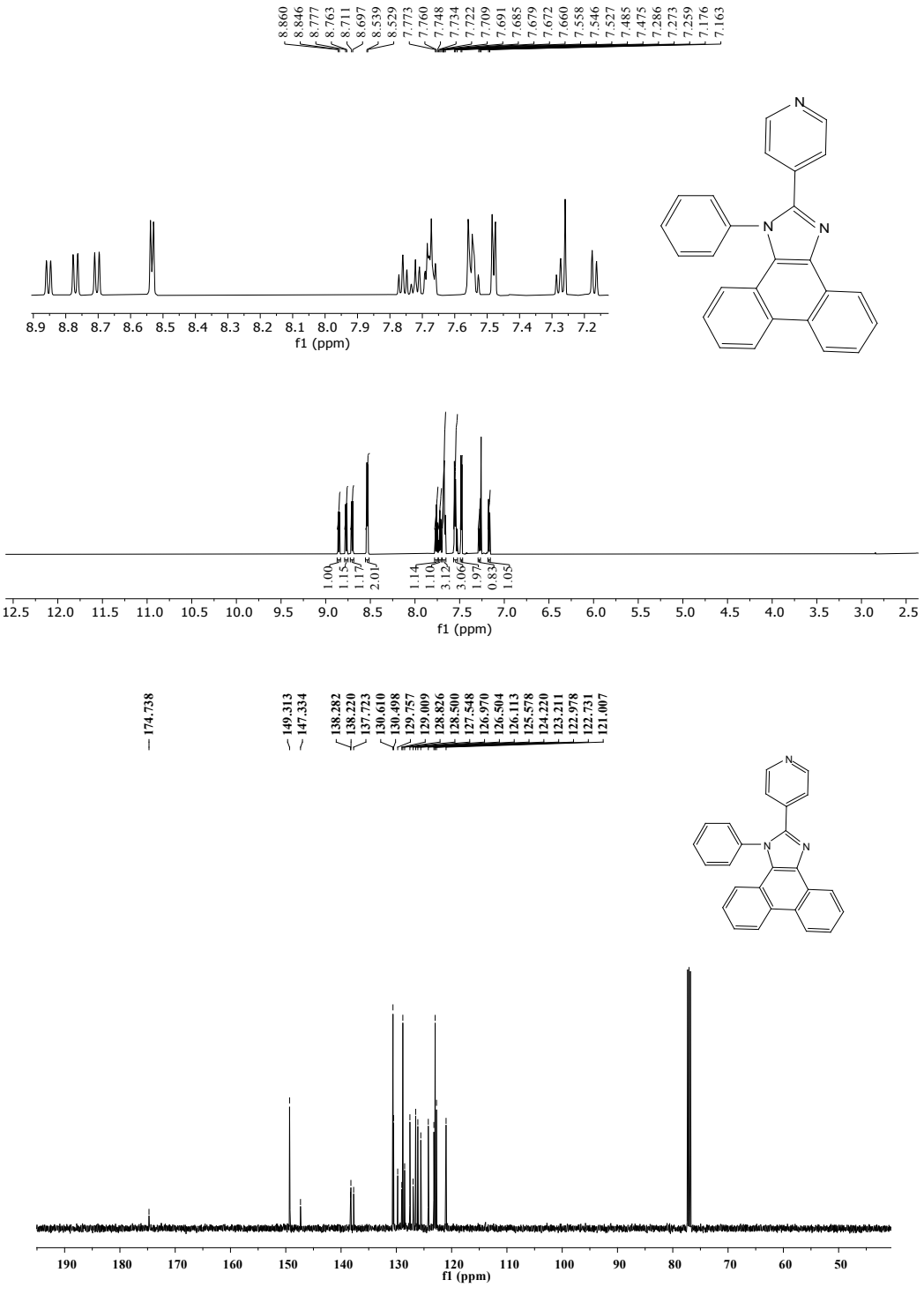

Figure SI 6: ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **2** in $CDCl_3$

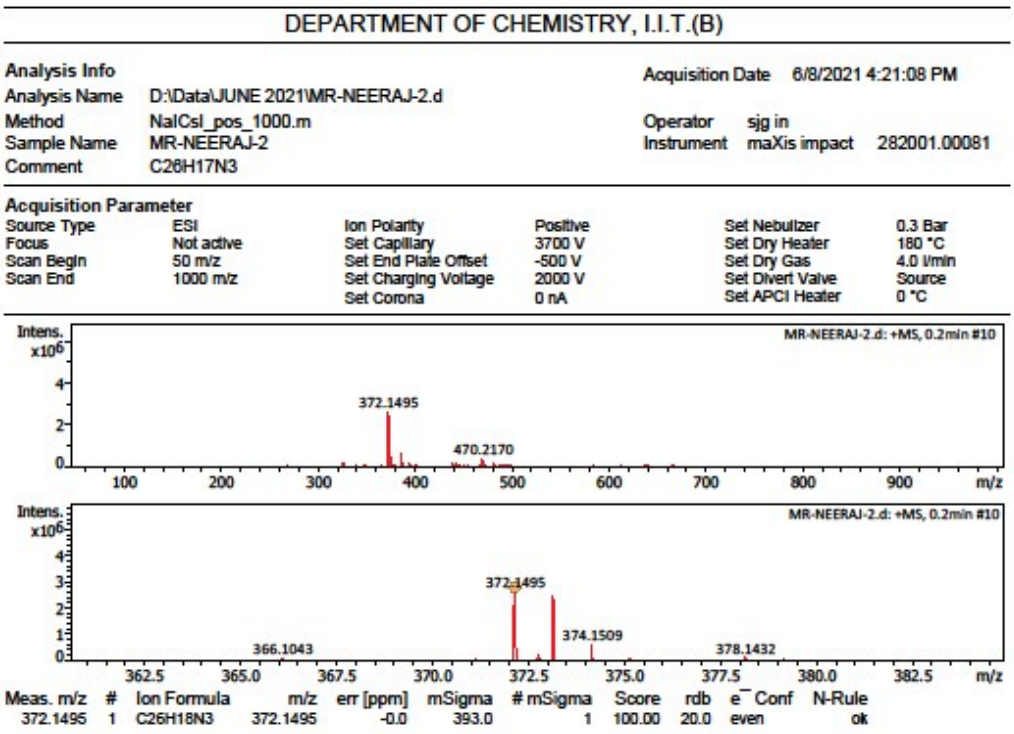

Figure SI 7: HRMS spectrum for **2.**

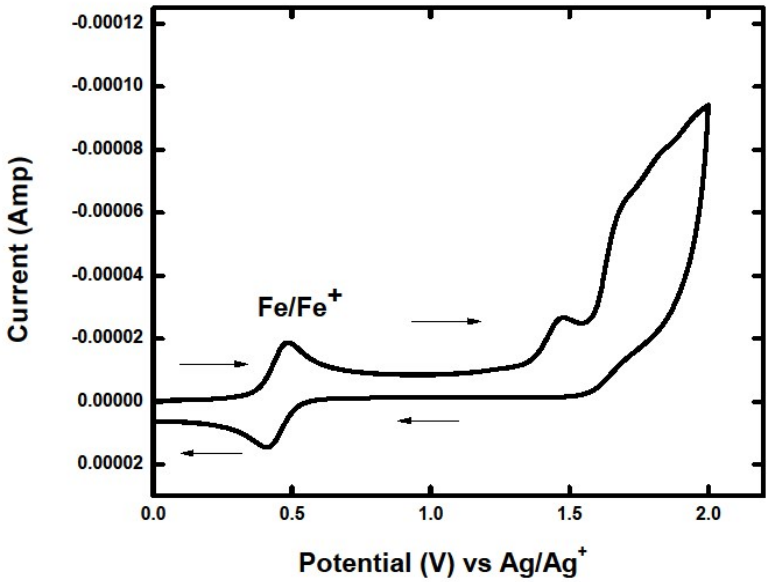

Figure SI 8: Cyclic voltammogram of **2**

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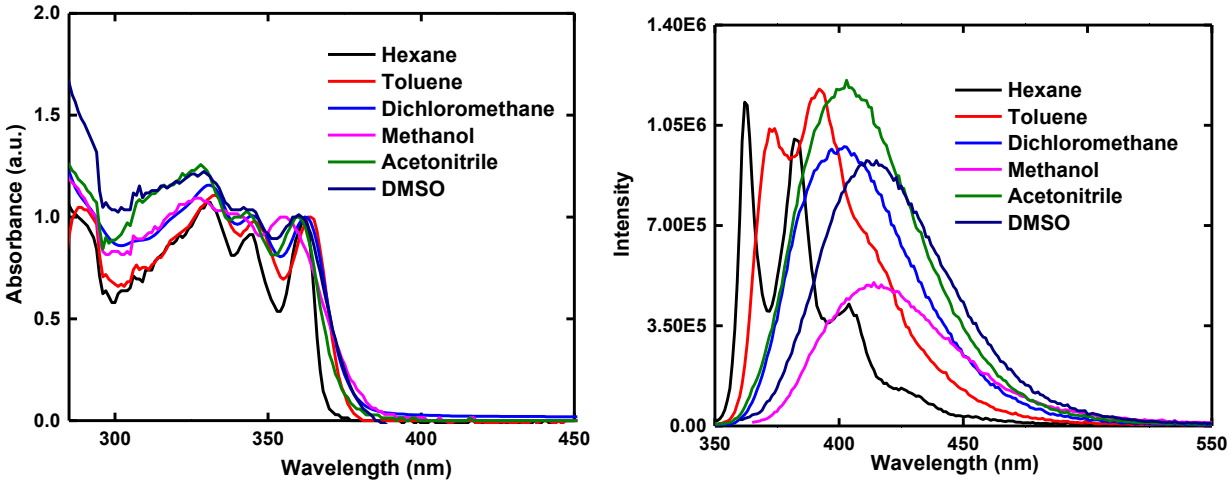


Figure SI 9: Absorption and emission spectra of **2** in different solvents

Table SI 3: Absorption and emission data of **2** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	361(4.05), 344(4.01), 329(4.07), 259(4.55)	381, 402	2830	71	3.37
Toluene	363(4.14), 345(4.12), 332(4.18)	373, 391	1970	73	3.35
DCM	362(4.78), 345(3.82), 331(4.85)	396	2370	72	3.34
CH_3OH	355(4.02), 326(4.06), 257(4.68)	415	4070	83	3.32
CH_3CN	360(4.06), 345(4.06), 328(4.14), 258(4.71)	408	3270	84	3.35
DMSO	360(4.14), 342(4.15), 329(4.22)	414	3620	89	3.33

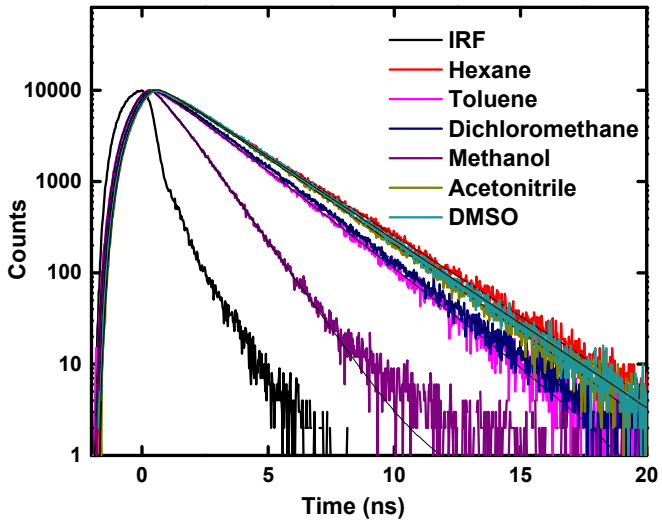
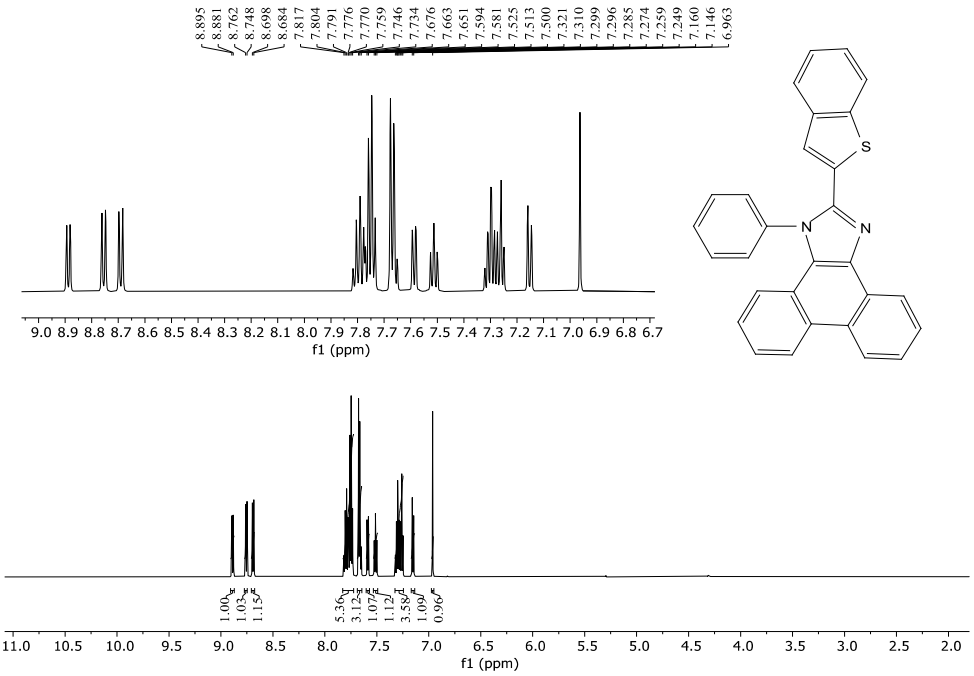


Figure SI 10: Fluorescence decay spectra of **2** in different solvents

Table SI 4: Fluorescence decay data of **2** in different solvents

Solvent	λ_{em}(nm)	τ(ns)	α	Chi sq.
Hexane	402	2.43,	100	1.00
Toluene	391	2.03	100	1.27
DCM	396	2.11	100	1.05
CH_3OH	415	1.07	100	1.02
CH_3CN	408	2.23	100	1.00
DMSO	414	2.37	100	1.12

Characterization and Spectroscopic data of 3



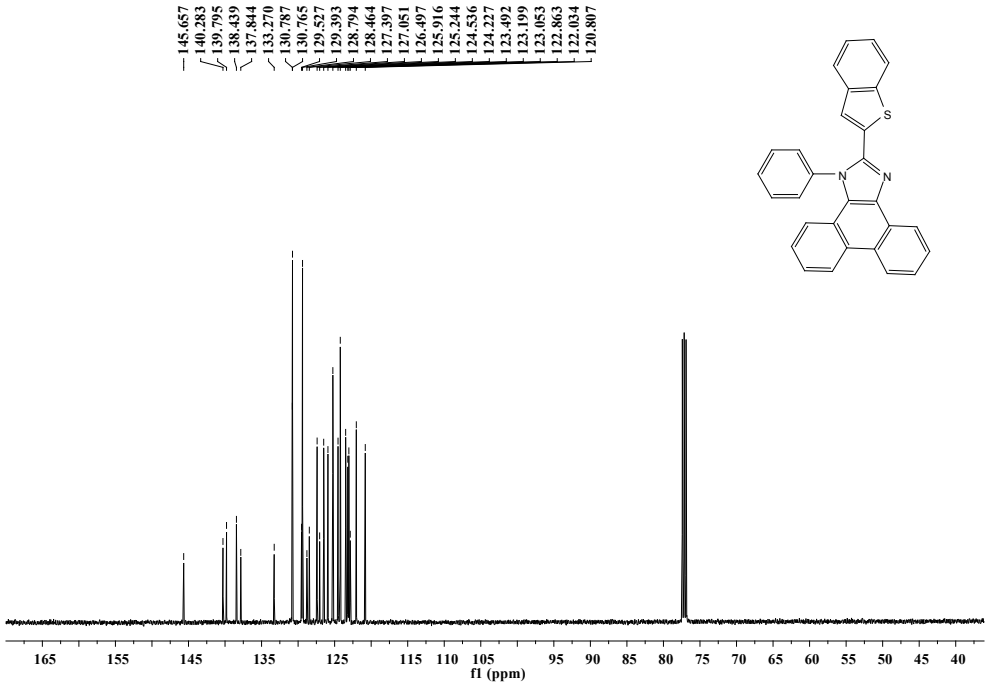


Figure SI 11: ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **3** in $CDCl_3$

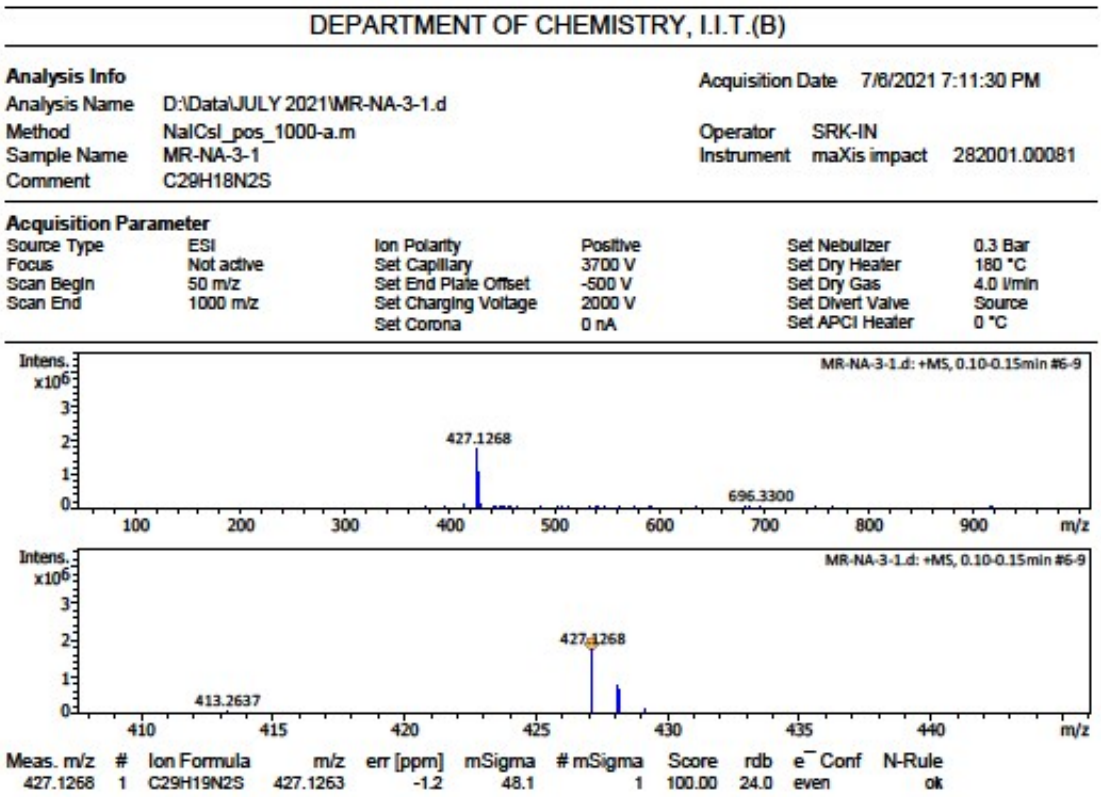


Figure SI 12: HRMS spectrum of **3.**

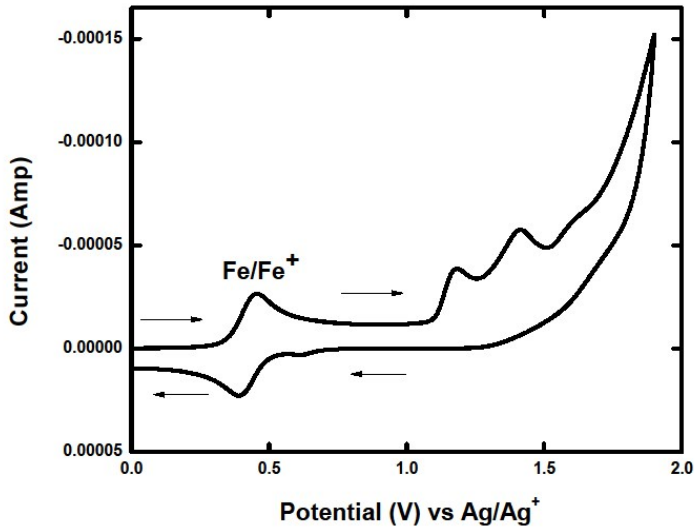


Figure SI 13: Cyclic voltammogram of **3**

Photophysical studies:

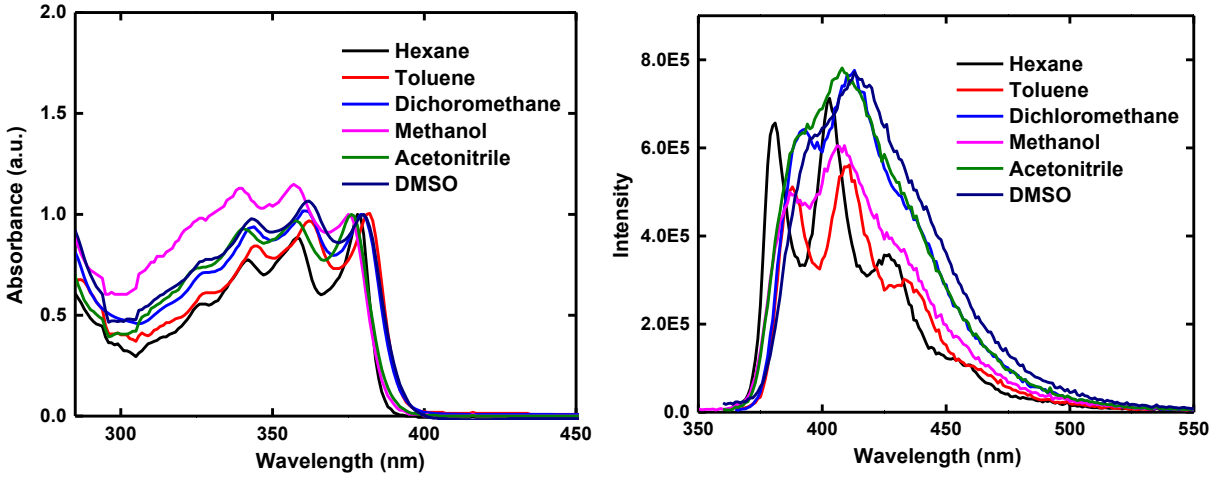


Figure SI 14: Absorption and emission spectra of **3** in different solvents

Table SI 5: Absorption and emission data of **3** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	378(5.45), 358(5.41), 342(5.36) 325(5.20), 262(5.63)	381, 403, 427.	1640	55	3.26
Toluene	381(5.56), 362(5.54), 344(5.48),286(5.38)	387, 410	1920	68	3.25
DCM	379(6.19), 361(6.20), 343(6.17), 263(6.33)	391, 411	2050	64	3.21
CH_3OH	375(5.23), 357(5.29), 339(5.28), 259(5.58)	387, 407	2090	68	3.26
CH_3CN	376(5.56), 357(5.54), 339(5.52), 325(5.42), 261(5.76)	407	2020	72	3.24
DMSO	379(5.73), 361(5.76), 343(5.71)	414	2230	73	3.33

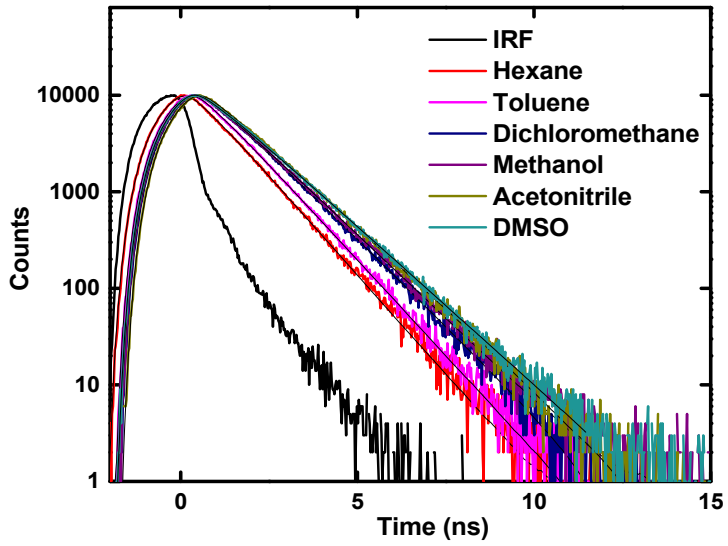


Figure SI 15: Fluorescence decay spectra of **3** in different solvents

Table SI 6: Fluorescence decay data of **3** in different solvents

Solvent	λ_{em}(nm)	τ(ns)	α	Chi sq.
Hexane	427.	1.00	100	1.01
Toluene	410	1.06	100	1.07
DCM	411	1.18	100	1.05
CH_3OH	407	1.22	100	1.00
CH_3CN	407	1.26	100	1.08
DMSO	414	1.30	100	1.00

Characterization and Spectroscopic data of 4

NMR:

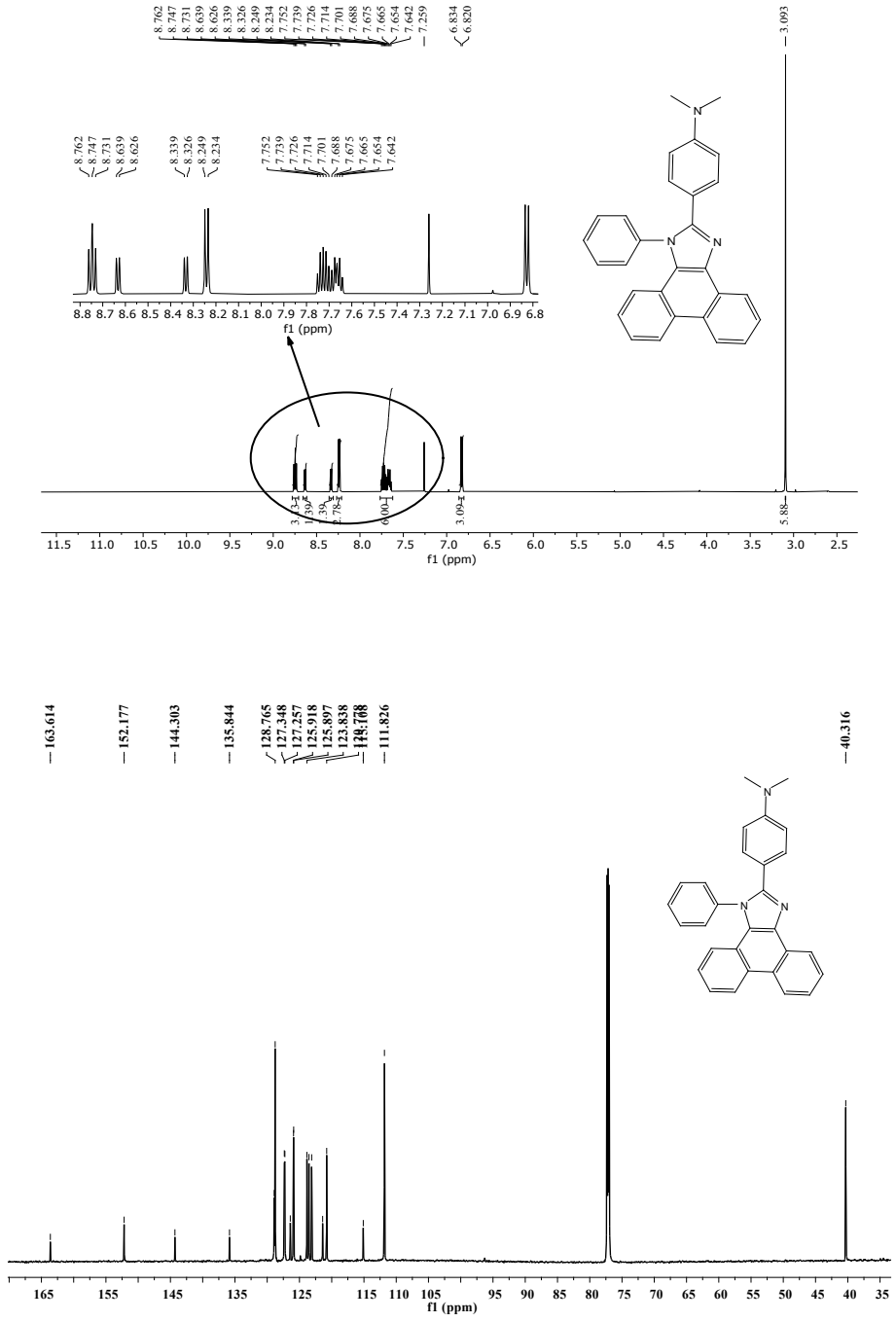


Figure SI 16: ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **4** in $CDCl_3$

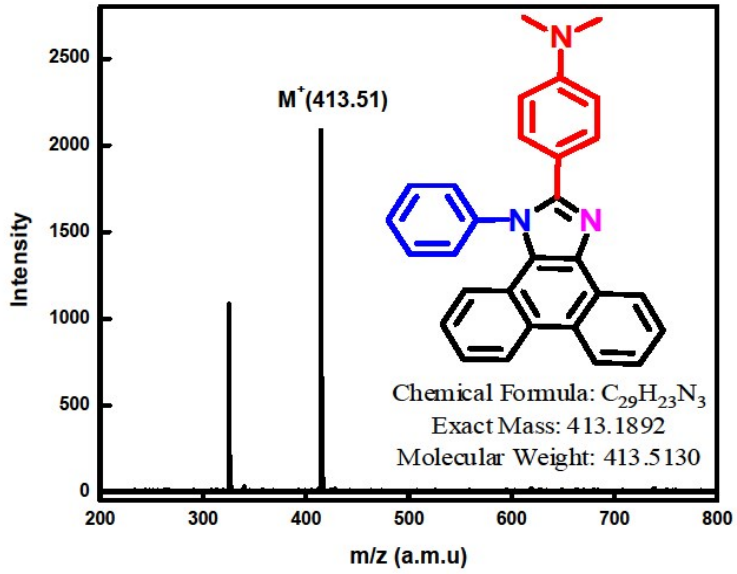


Figure SI 17: MALDI-TOF spectrum of **4**

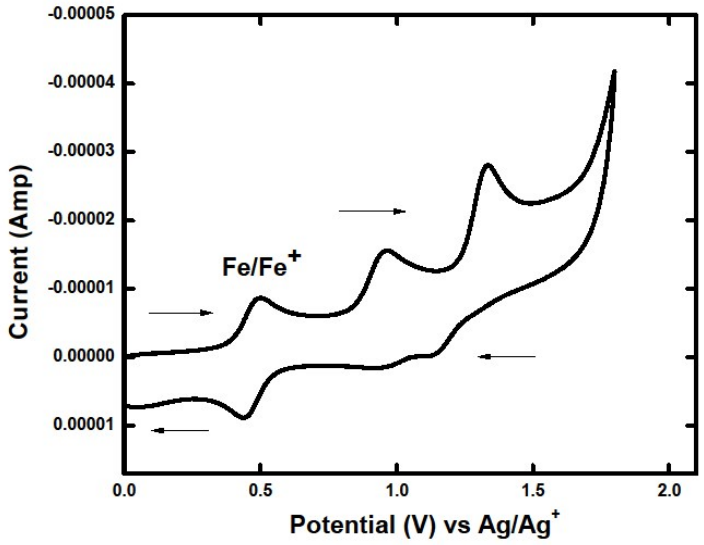


Figure SI 18: Cyclic voltammogram of **4.**

Photophysical studies:

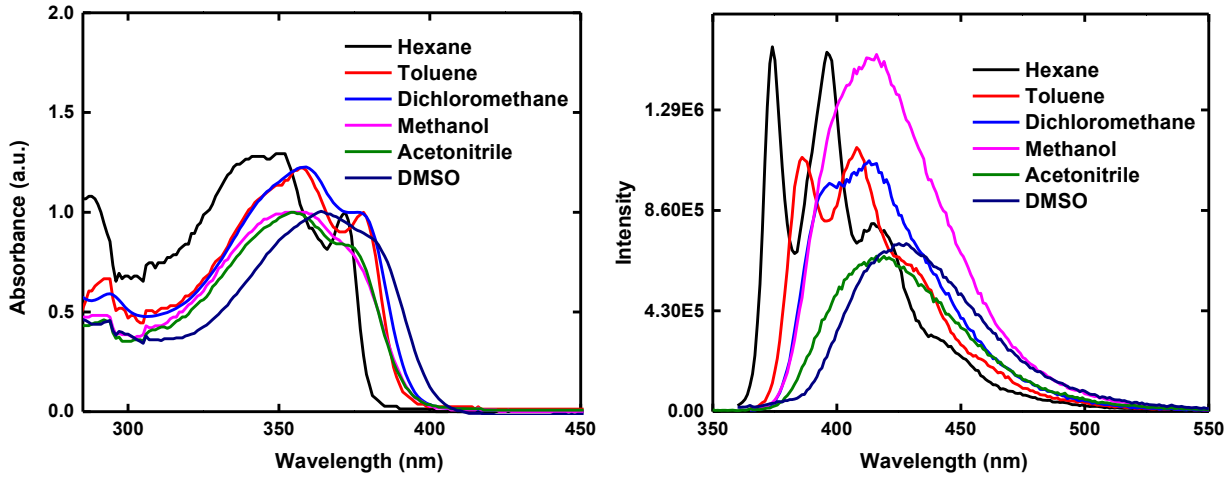


Figure SI 19: Absorption and emission spectra of **4** in different solvents

Table SI 7: Absorption and emission data of **4** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	371(4.40), 346(4.51), 279(3.46), 257(4.65)	373, 396	1700	98	3.34
Toluene	378(4.45), 357(4.53), 292(4.27)	386, 407.	1880	86	3.31
DCM	379(4.29), 359(5.39), 261(5.40)	396, 411	2050	90	3.20
CH_3OH	355(4.58), 258(4.63)	413	3950	94	3.20
CH_3CN	355(4.67), 258(4.66)	417	4180	87	3.19
DMSO	369(4.89)	429	3790	93	3.35

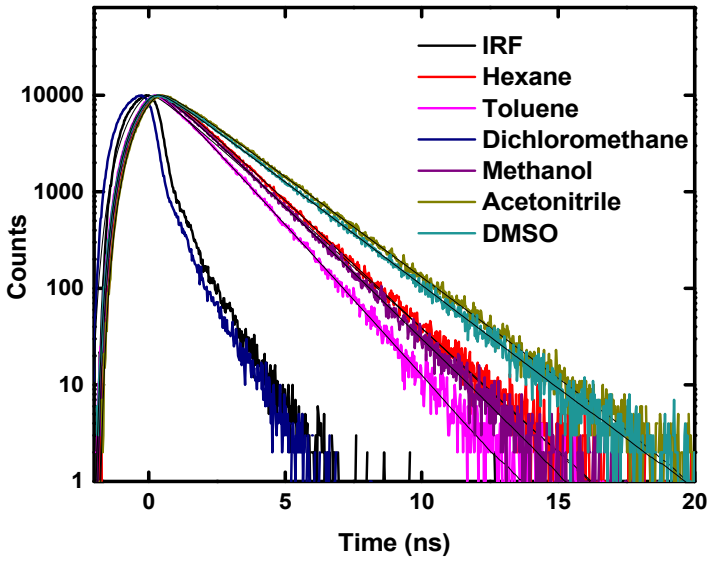


Figure SI 20: Fluorescence decay spectra of **4** in different solvents

Table SI 8: Fluorescence decay data of **4** in different solvents

Solvent	λ_{em}(nm)	τ(ns)	α	Chi sq.
Hexane	396	1.63.	100.	1.00
Toluene	407.	1.37	100	1.09
DCM	411	1.58	100	1.05
CH_3OH	413	1.59	100	1.02
CH_3CN	417	2.08	100	1.04
DMSO	429	2.02	100	1.01

Characterization and Spectroscopic data of 5

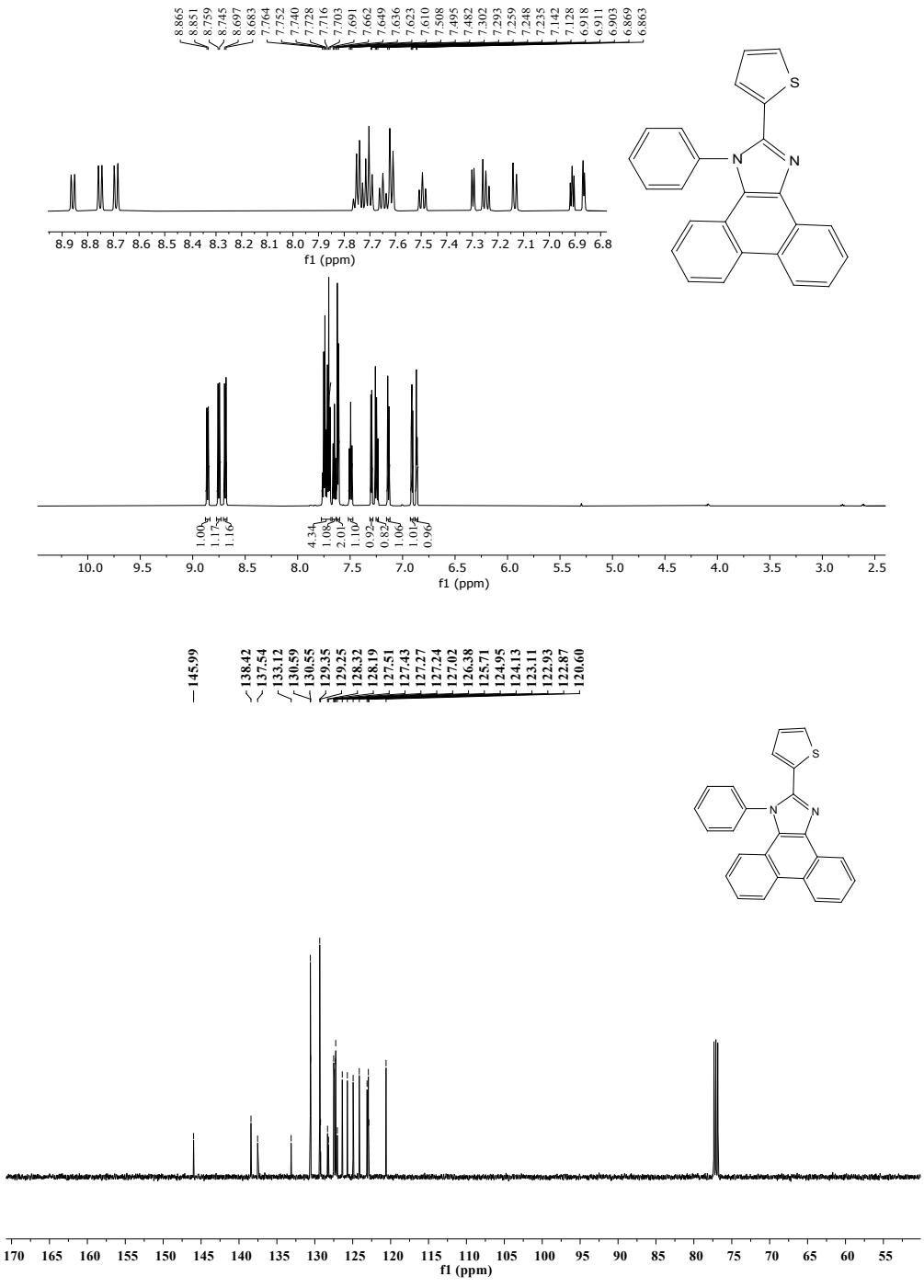


Figure SI 21: ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of **5** in $CDCl_3$

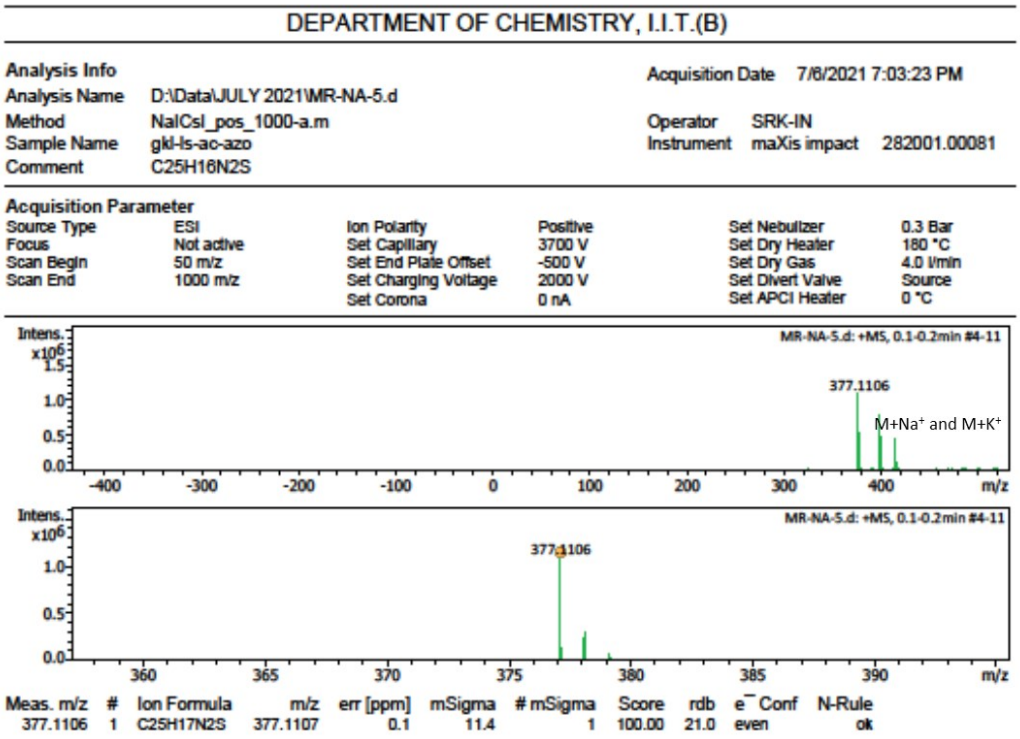


Figure SI 22: HRMS spectrum of **5.**

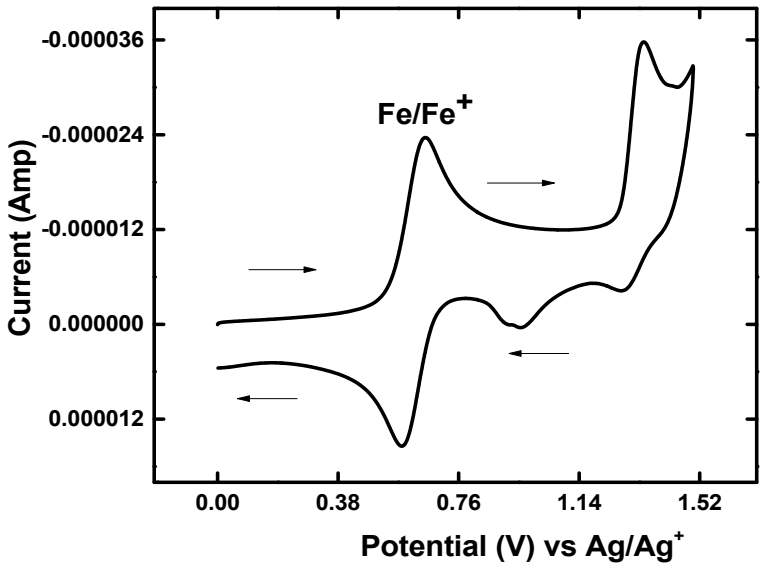


Figure SI 23: Cyclic voltammogram of **5.**

Photophysical studies:

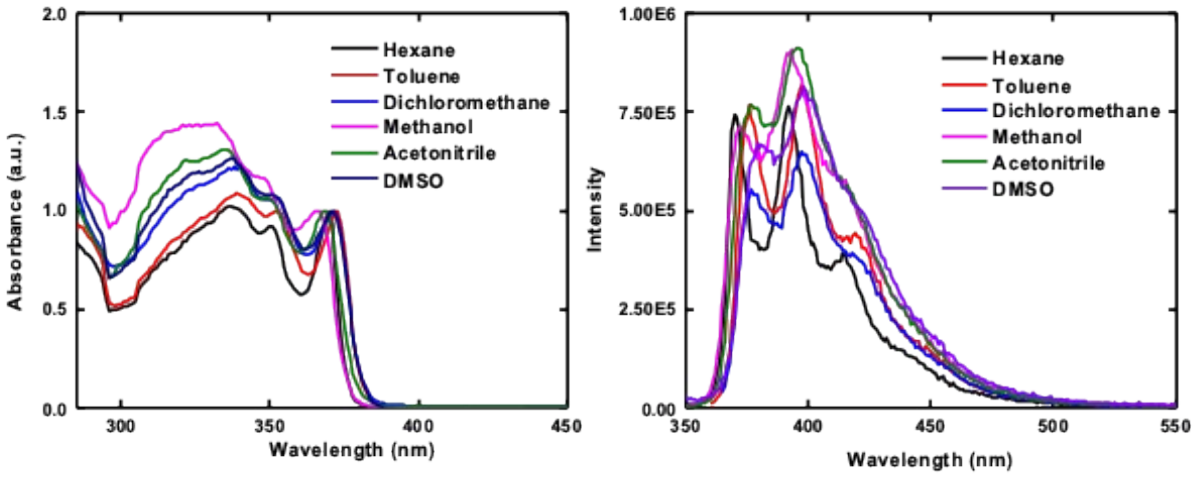


Figure SI 24: Absorption and emission spectra of **5** in different solvents

Table SI 9: Absorption and emission data of **5** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	369(4.63), 350(4.60), 337(4.64), 263(4.99)	371, 392, 414.	1590	48	3.37
Toluene	372(3.98), 353(4.65), 339(4.69), 285(4.63)	376, 397	1700	58	3.30
DCM	371(5.25), 352(5.27), 338(5.34), 263(5.53)	376, 397	1770	53	3.30
CH_3OH	366(4.31), 347(4.37), 325(4.46), 260(4.92)	372,393	1880	53	3.38
CH_3CN	368(4.60), 349(4.63), 332(4.71), 261(5.10)	376, 395, 413	1860	53	3.35
DMSO	372(4.67), 353(4.70), 336(4.77), 264(5.20)	394	1500	57	3.35

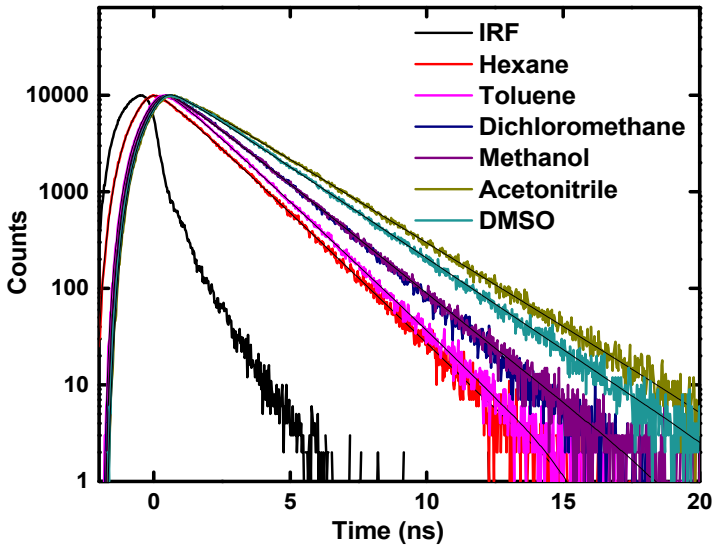


Figure SI 25: Fluorescence decay spectra of **5** in different solvents

Table SI 10: Fluorescence decay data of **5** in different solvents

Solvent	λ_{em} (nm)	τ(ns)	α	Chi sq.
Hexane	392	1.60	100.	1.05
Toluene	397	1.62	100	1.05
DCM	397	1.90	100	1.05
CH_3OH	393	1.91	100	1.08
CH_3CN	395	2.52	100	1.09
DMSO	394	2.29	100	1.15

Characterization and Spectroscopic data of 6

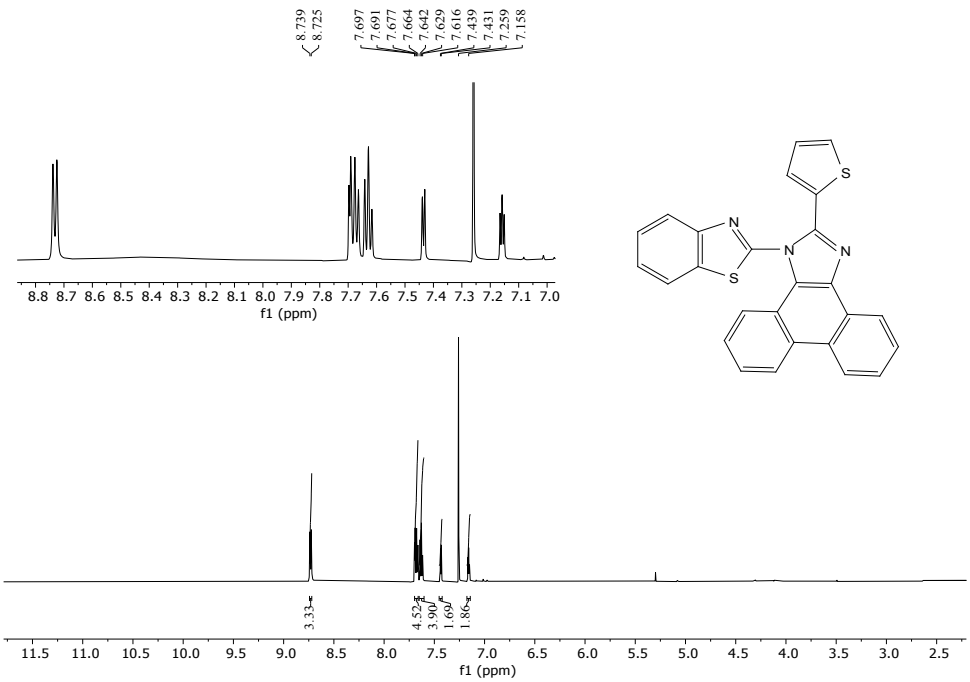


Figure SI 26: ^{1}H NMR spectra of **6**in $CDCl_3$

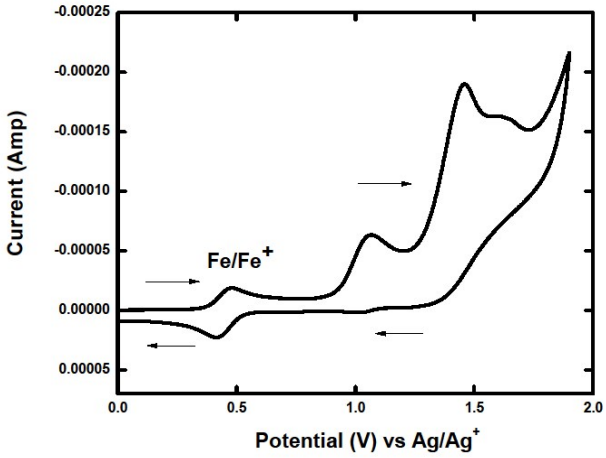


Figure SI 27: Cyclic voltammetry of **6.**

Photophysical studies:

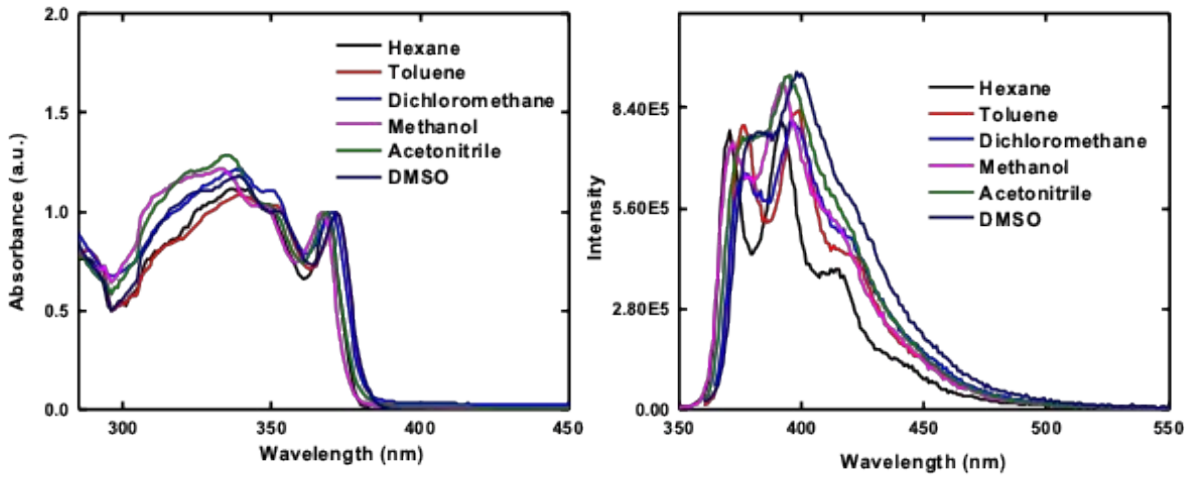


Figure SI 28: Absorption and emission spectra of **6** in different solvents

Table SI 11: Absorption and emission data of **6** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	369(4.11), 337(5.16), 262(6.91)	371, 391, 414	1530	51	3.38
Toluene	372(5.63), 339(5.67), 288(5.54)	376, 397	1700	65	3.34
DCM	370(6.25),338(6.34), 258(6.48)	376, 396	1770	54	3.31
CH_3OH	367(5.62), 348(5.64), 331(6.13), 261(6.09)	373, 392	1730	66	3.38
CH_3CN	368(5.45), 349(5.46), 325(5.56), 262(5.88), 255(5.82)	376, 395	1860	56	3.36
DMSO	372(5.85), 352(5.86), 338(5.92), 265(6.30)	396	1630	68	3.31

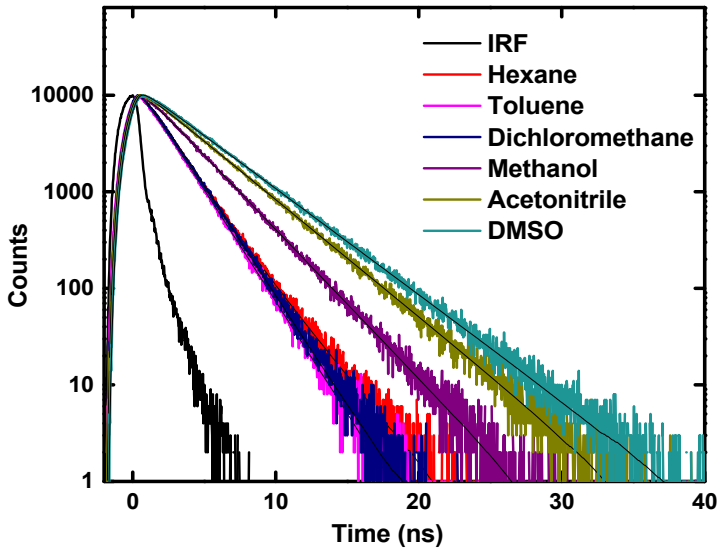


Figure SI 29: Fluorescence decay spectra of **6** in different solvents

Table SI 12: Fluorescence decay data of **6** in different solvents

Solvent	λ_{em} (nm)	τ_1 (ns)	α	Chi sq
Hexane	414.	1.59	100	1.00
Toluene	397	1.87.	100	1.09
DCM	396	1.90	100	1.18
CH_3OH	392	2.82	100	1.06
CH_3CN	395	3.58	100	1.02
DMSO	396	3.95	100	1.09

Characterization and Spectroscopic data of 7

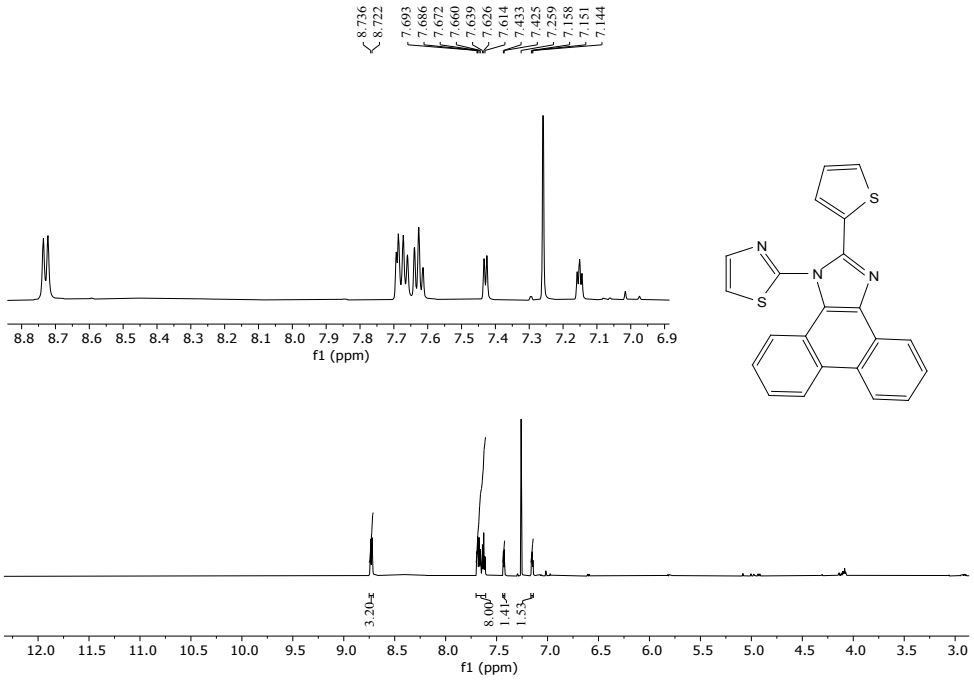


Figure SI 30: ^{1}H NMR spectrum of **7** in $CDCl_3$

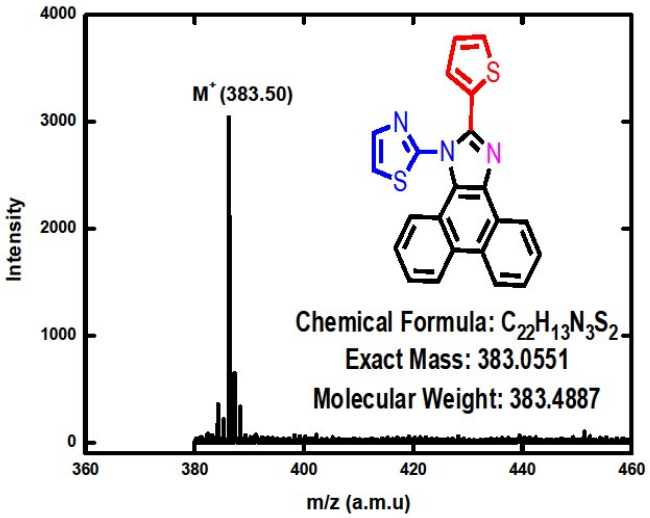


Figure SI 31: MALDI-TOF spectrum of **7.**

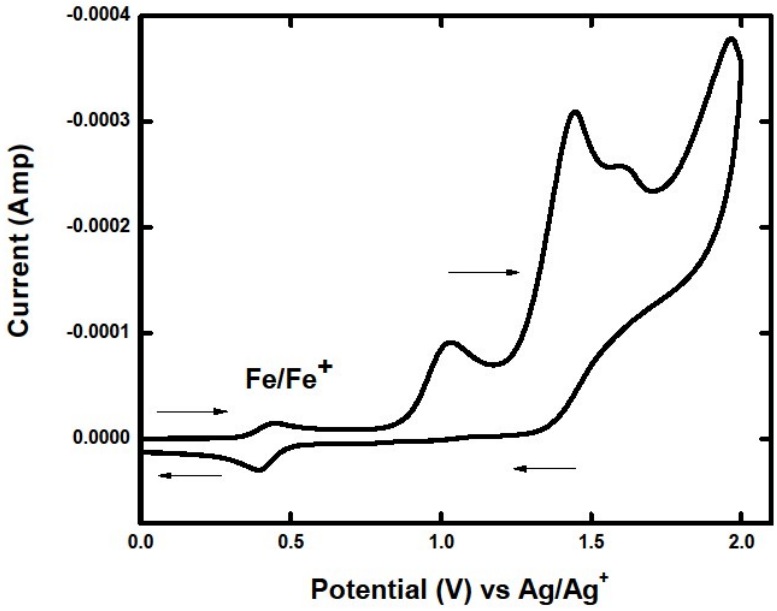


Figure SI 32: Cyclic voltammogram of **7.**

Photophysical studies:

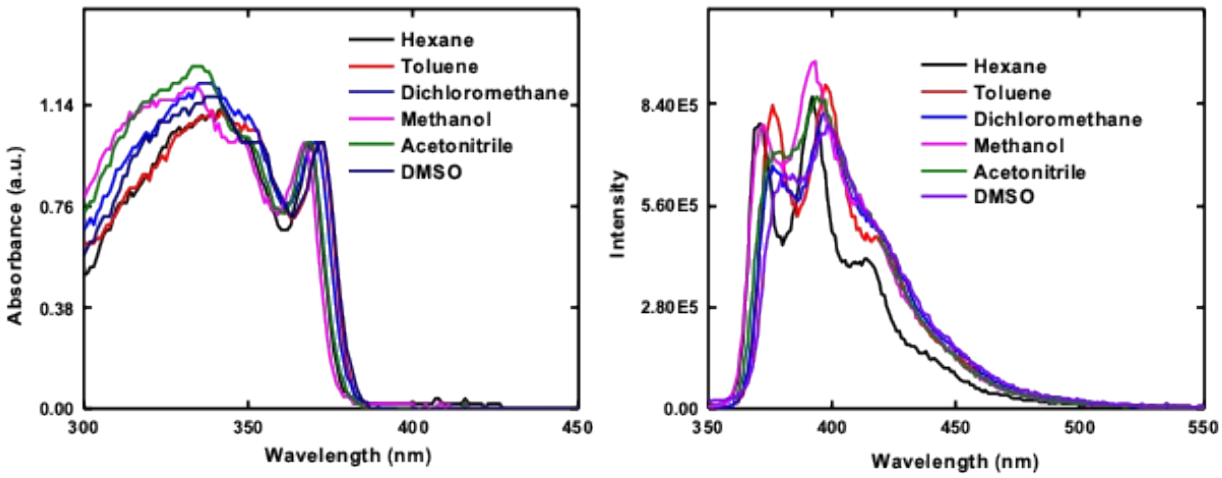


Figure SI 33: Absorption and emission spectra of **7** in different solvents

Table SI 13: Absorption and emission data of **7** in different solvents

Solvent	λ_{abs} [nm], (log ε)	λ_{em} (nm)	Stoke shift (cm^{-1})	Φ_F	Eg (eV)
Hexane	372(4.93), 341(4.98), 286(5.23), 263(5.33)	373, 396, 416	1629	48	3.33
Toluene	372(5.08), 338(5.12), 291(5.02)	376, 396.	1629	62	3.31
DCM	370(5.95), 337(6.03), 264(6.41)	375, 396	1774	50	3.34
CH_3OH	368(4.97), 327(5.07), 261(5.46)	371, 391	1598	61	3.37
CH_3CN	368(4.90), 328(5.02), 262(5.47)	377, 394	1793	56	3.36
DMSO	372(5.29), 330(5.36)	394	1501	63	3.36

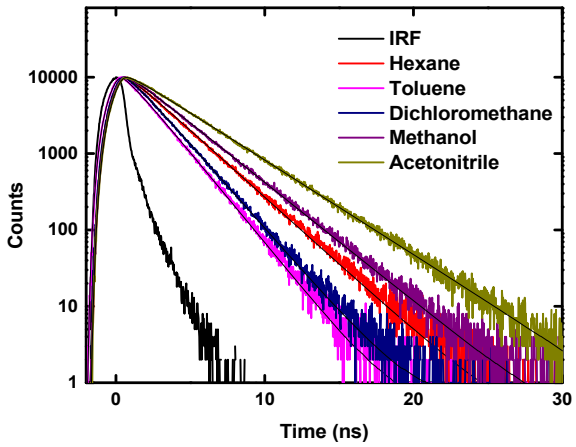


Figure SI 34: Fluorescence decay spectra of **7** in different solvents

Table SI 14: Fluorescence decay data of **7** in different solvents

Solvent	λ_{em} (nm)	τ_1 (ns)	α	Chi sq
Hexane	416	1.83	100	1.06
Toluene	396	1.96	100	1.20
DCM	396	1.83	100	1.07
CH_3OH	391	2.79	100	1.00
CH_3CN	394	3.51	100	1.01
DMSO	394		100	

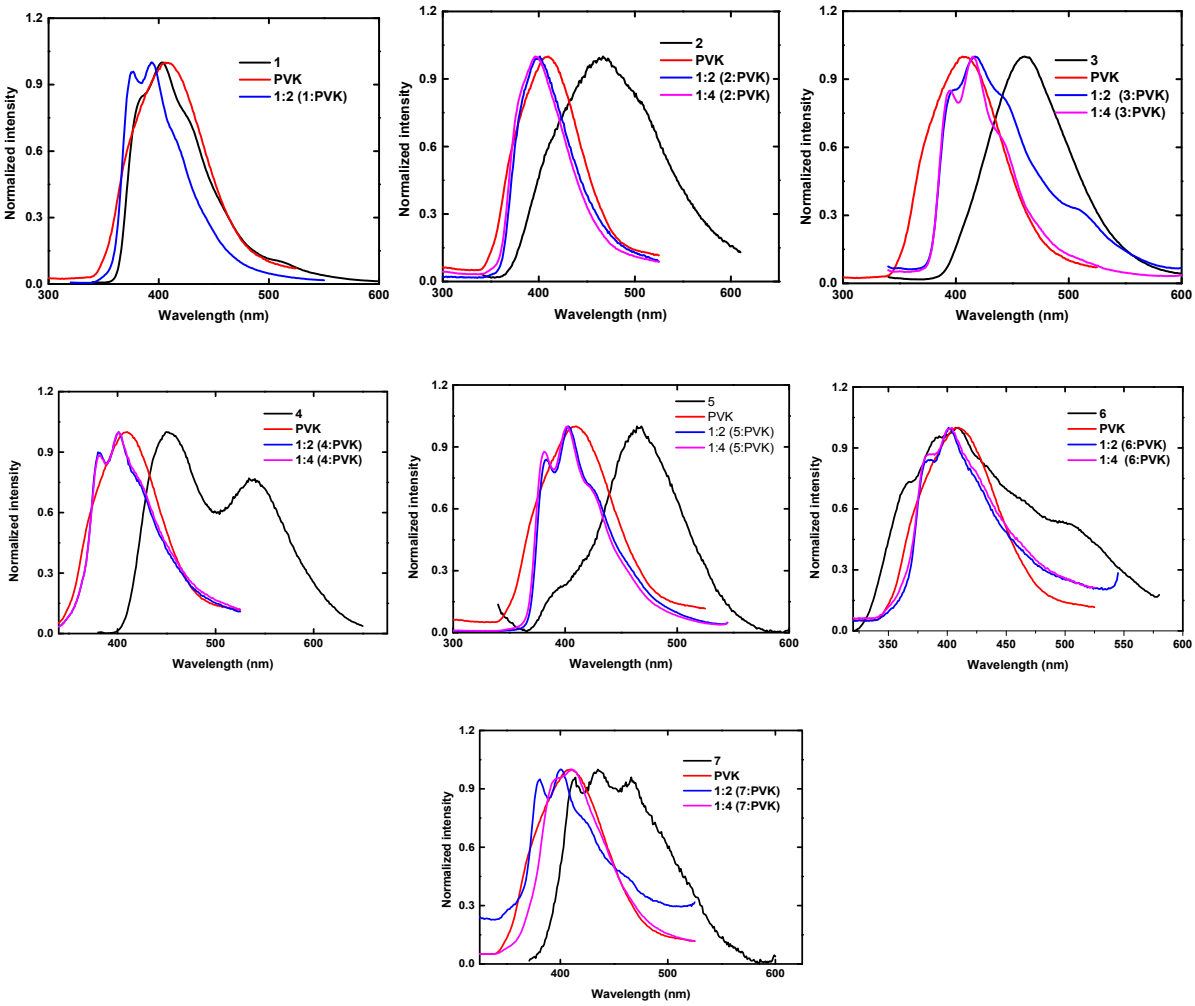


Figure SI 35: Emission spectra in thin films of **1-7**, PVK and their blends

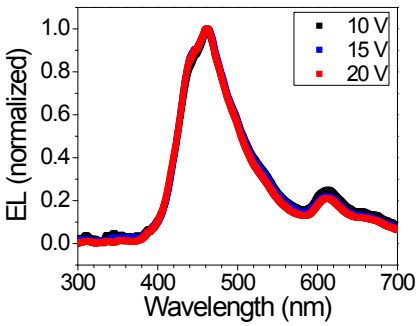


Figure SI 36: Electroluminescence of OLEDs fabricated from **5** at different driving voltage