Supporting information

Photo-physical Properties of Salts of a Di-topic Imidazole-Tethered Anthracene Derivative in Solid and Solution

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Spectroscopic data of the salts:

Salt **H_2L.2-NBA**: Isolated Yield: 65 %. Melting 171°C. HRMS calculated for $C_{21}H_{22}N_3$ (m^+) 316.1814; found 316.1847. ^{1}H-NMR (600 MHz, DMSO-d_6): 8.69 (s, 1H), 8.48 (d, J = 6 Hz, 2H), 8.15 (d, J = 6 Hz, 2H), 7.74 (d, J = 6 Hz, 1H), 7.68 (t, J = 6 Hz, 1H), 7.64-7.61 (m, 4H), 7.58-7.52 (m, 3H), 7.15 (s, 1H), 6.90 (s, 1H), 5.00 (s, 2H), 4.08 (t, J = 6 Hz, 2H), 3.03 (m, 2H), 2.08 (m, 2H). IR (KBr, cm^{-1}): 3417 (br, w), 3137 (w), 2943 (w), 2831 (w), 1626 (s), 1590 (m), 1570 (m), 1520 (s), 1471 (w), 1442 (w), 1375 (s), 1355 (s), 1279 (m), 1225 (m), 1189 (w), 1159 (w), 1076 (s), 1049 (w), 1030 (w), 963 (w), 892 (m), 831 (s), 785 (s), 733 (s), 663 (m), 644 (m).

Salt **H_2L.2,3-H_2DHBA**: Isolated Yield: 69 %. Melting 201°C. HRMS calculated for $C_{21}H_{22}N_3$ (m^+) 316.1814; found 316.1843. ^{1}H-NMR (600 MHz, DMSO-d_6): 8.76 (s, 1H), 8.50 (d, J = 12 Hz, 2H), 8.28 (s, 1H), 8.18 (d, J = 6 Hz, 2H), 7.68 (m, 3H), 7.61 (t, J = 6 Hz, 2H), 7.19 (s, 1H), 7.11 (d, J = 6 Hz, 1H), 6.95 (s, 1H), 6.69 (d, J = 6 Hz, 1H), 6.41 (t, J = 6 Hz, 1H), 5.15 (s, 2H), 4.11 (t, J = 6 Hz, 2H), 3.18 (m, 2H), 2.15 (m, 2H). IR (KBr, cm^{-1}): 3434 (br, w), 3132 (w), 3036 (w), 2838 (w), 1634 (s), 1560 (s), 1505 (s), 1468 (w), 1450 (w), 1392 (s), 1341 (w), 1274 (s), 1266 (s), 1232 (w), 1193 (w), 1152 (w), 1082 (s), 1067 (w), 996 (m), 920 (s), 890 (w), 826 (m), 783 (s), 735 (s), 661 (m), 632 (m).

Salt **H_2L.2,4-DNP**: Isolated Yield: 63 %. Melting 144°C. HRMS calculated for $C_{21}H_{22}N_3$ (m^+) 316.1814; found 316.1832. ^{1}H-NMR (600 MHz, DMSO-d_6): 8.78 (s, 1H), 8.59 (d, J = 6 Hz, 1H), 8.49 (d, J = 12 Hz, 2H), 8.20 (d, J = 6 Hz, 2H), 7.79 (d, J = 6 Hz, 1H), 7.72 (m, 3H), 7.63 (t, J = 6 Hz, 2H), 7.22 (s, 1H), 6.98 (s, 1H), 6.32 (m, 1H), 5.20 (s, 2H), 4.12 (t, J = 6 Hz, 2H), 3.24 (m, 2H), 2.15 (m, 2H). IR (KBr, cm^{-1}): 3431 (br, w), 3051 (w), 2960 (w), 2779 (w), 1624 (w),

1590 (s), 1558 (m), 1519 (s), 1467 (s), 1305 (m), 1283 (m), 1233 (m), 1130 (s), 1074 (w), 1060 (w), 985 (w), 920 (w), 887 (m), 828 (s), 789 (w), 730 (s), 684 (m), 636 (m).

Salt **H_2L.2,4,6-TNP**: Isolated Yield: 65 %. Melting 157 °C. HRMS calculated for $C_{21}H_{22}N_3$ (m^+) 316.1814; found 316.1814. ^{1}H-NMR (400 MHz, DMSO-d_6): 8.79 (s, 1H), 8.58 (s, 2H), 8.47 (d, J = 8 Hz, 2H), 8.20 (d, J = 8 Hz, 2H), 7.81 (s, 1H), 7.72 (t, J = 8 Hz, 2H), 7.64 (d, J = 8 Hz, 2H), 7.25 (s, 1H), 7.02 (s, 1H), 5.21 (s, 2H), 4.12 (t, J = 8 Hz, 2H), 3.27 (t, J = 8 Hz, 2H), 2.20 (p, J = 8 Hz, 2H). IR (KBr, cm^{-1}): 3459 (br, w), 3154 (w), 3053 (w), 2964 (w), 1631 (w), 1610 (m), 1557 (s), 1490 (w), 1364 (m), 1317 (s), 1266 (s), 1161 (m), 1080 (m), 1023 (w), 912 (w), 787 (m), 730 (m), 709 (m), 636 (m).

Cocrystal **H_2L.4-NP.4-HNP**: Isolated Yield: 67 %. Melting 127 °C. HRMS calculated for $C_{21}H_{22}N_3$ (m^+) 316.1814; found 316.1846. ^{1}H-NMR (600 MHz, DMSO-d_6): 8.56 (s, 1H), 8.42 (d, J = 12 Hz, 2H), 8.12 (m, 6H), 7.59 (d, J = 6 Hz, 2H), 7.54 (m, 3H), 7.09 (s, 3H), 6.91 (d, J = 12 Hz, 4H), 6.85 (s, 1H), 4.65 (s, 2H), 4.02 (t, J = 6 Hz, 2H), 2.75 (m, 2H), 1.94 (m, 2H). IR (KBr, cm^{-1}): 3436 (br, w), 3116 (w), 3053 (w), 2873 (w), 1629 (w), 1576 (s), 1511 (w), 1488 (m), 1471 (m), 1396 (m), 1329 (s), 1292 (m), 1251 (m), 1161 (s), 1106 (s), 1080 (w), 1051 (w), 988 (m), 927 (m), 891 (m), 848 (s), 790 (w), 729 (s), 664 (m), 639 (s).

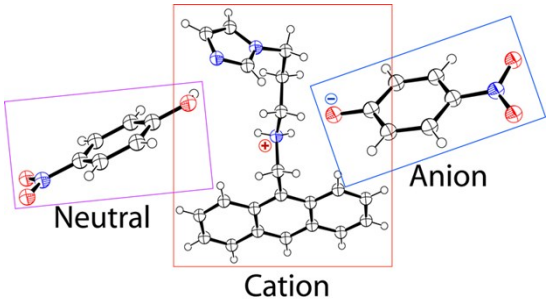


Figure S1: ORTEP of cocrystal of of 4-nitrophenol with HL

Table S1: Hydrogen bond parameters of different salts of **HL**.

Salts	D-H···A	d_{D-H} (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	∠D-H···A (°)
H_2L.4-NP.4-HNP	O(3)-H(3)···N(1) [x, y, -1+z]	0.82(2)	1.87(2)	2.678(3)	171(2)
	N(3)-H(3A)···O(4) [x, y, -1+z]	0.89(3)	1.88(3)	2.694(2)	151(3)
	N(3)-H(3B)···O(4) [1-x, 1-y, 1-z]	0.89(3)	1.79(3)	2.670(2)	168(2)
	C(2)-H(2B)···O(6) [1-x, -y, 1-z]	0.97(6)	2.58(4)	3.226(3)	124(2)
	C(3)-H(3C)···O(2) [x, y, z]	0.97(3)	2.51(3)	3.402(4	153(3)
H_2L.2,4-DNP	N(3)-H(3D)···O(1) [1-x, 1-y, 1-z]	0.94(3)	1.85(3)	2.778(3)	170(3)
	N(3)-H(4D)···O(1) [x, y, z]	1.02(3)	1.80(3)	2.768(3)	156(3)
	N(3)-H(4D)···O(1) [x, y, z]	1.02(3)	2.33(4)	2.977(4)	120(2)
	C(1)-H(1B)···O(2) [x, y, z]	0.97(2)	2.53(5)	2.951(4)	106(3)
	C(2)-H(2A)···O(2) [x, y, z]	0.97(3)	2.51(4)	3.128(4)	121(3)
H_2L.2,4,6-TNP	N(2)-H(2A)···N(1) [x, y, z]	0.89(3)	1.99(4)	2.859(3)	165(3)
	N(2)-H(2B)···O(1) [x, y, z]	0.89(3)	2.02(5)	2.692(3)	131(4)
	N(2)-H(2B)···O(2) [x, y, z]	0.89(3)	2.17(3)	2.907(4)	139(4)
H_2L.2-NBA	N(3)-H(3A)···O(1) [1-x, -y, 1-z]	0.89(3)	1.86(2)	2.740(2)	171(2)
	N(3)-H(3A)···O(2) [1-x, -y, 1-z]	0.89(3)	2.55(5)	3.187(2)	129(2)
	N(3)-H(3B)···O(1) [x, y, z]	0.89(3)	1.95(3)	2.745(2)	147(4)
	C(1)-H(1A)···O(2) [1+x, y, z]	0.97(2)	2.53(5)	3.313(2)	138(2)
	C(10)-H(10)···O(2) [1-x, -y, 1-z]	0.93(3)	2.49(3)	3.336(3)	151(4)
H_2L.2,3-H_2DHBA	N(3)-H(3A)···O(1) [x, y, z]	0.89(4)	1.84(6)	2.726(2)	173(5)
	N(3)-H(3A)···O(2) [x, y, z]	0.89(3)	2.52(4)	3.151(2)	128(2)
	N(3)-H(3B)···O(1) [1-x, 1-y, 1-z]	0.89(5)	1.94(3)	2.749(2)	151(4)
	O(4)-H(4)···N(1) [x, 1+y, -1+z]	0.82(2)	1.94(3)	2.744(3)	168(3)

Table S2: Energy details from DFT calculation using B3LYP/6functional using 31+G (d,p) as basis set.

Compounds	HOMO (eV)	LUMO (eV)	Energy difference = HOMO-LUMO (eV)	Optimized energy ($KJmol^{-1}$)
HL	-5.5326	-2.0628	-3.47	-2565640.5624
H_2L.4NP	-5.9026	-2.4378	-3.46	-3909954.943
H_2L.2,4,-DNP	-5.8670	-3.1118	-2.76	-4446877.56921
H_2L.2,4,6-TNP	-6.4300	-3.2174	-3.22	-4983802.33517
H_2L.2-NBA	-5.7854	-2.8337	-2.95	-4207511.570839
H_2L.2,3-H_2DHBA	-5.7002	-2.2359	-3.46	-4065671.20068

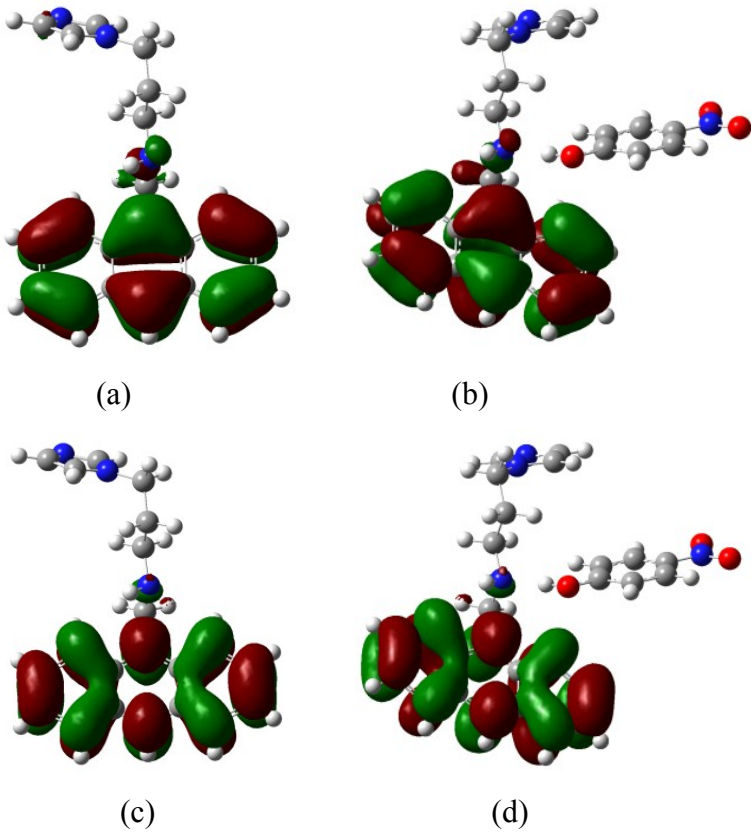


Figure S2: (a, b) HOMO and (c, d) LUMO of **HL** and **HL.4-NP.**

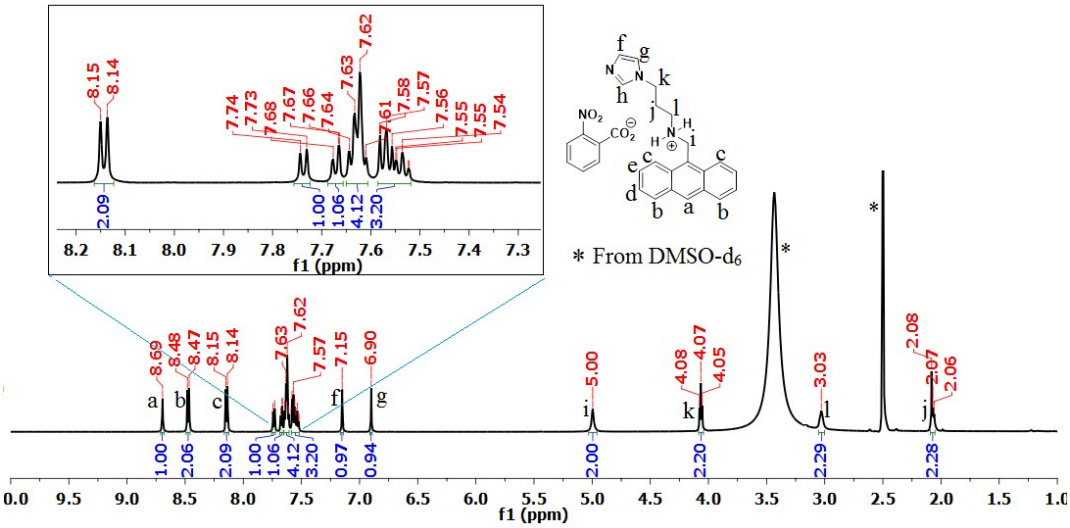


Figure S3: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of salt **H_2L.2-NBA**.

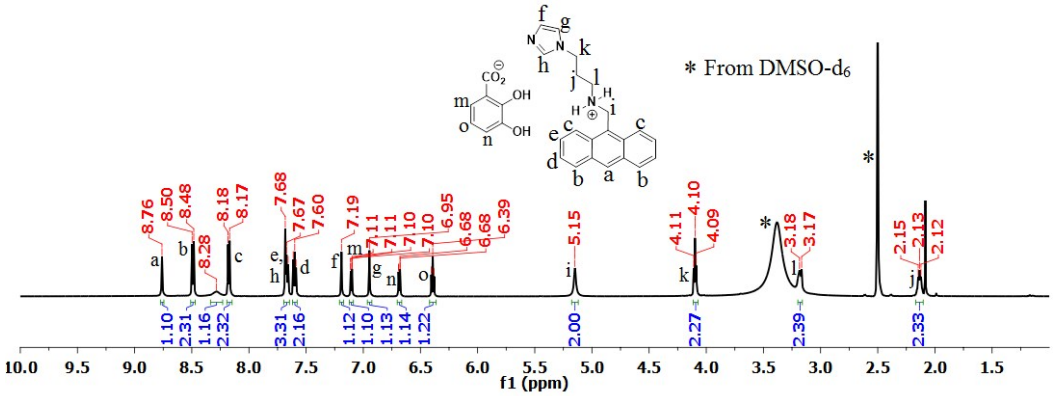


Figure S4: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of salt **H_2L.2,3-H_2DHBA**.

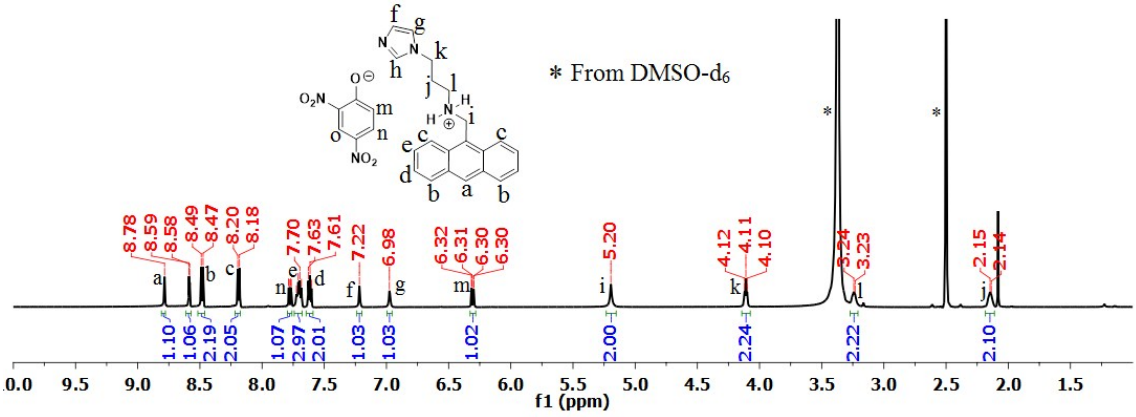


Figure S5: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of salt **H_2L.2,4-DNP**.

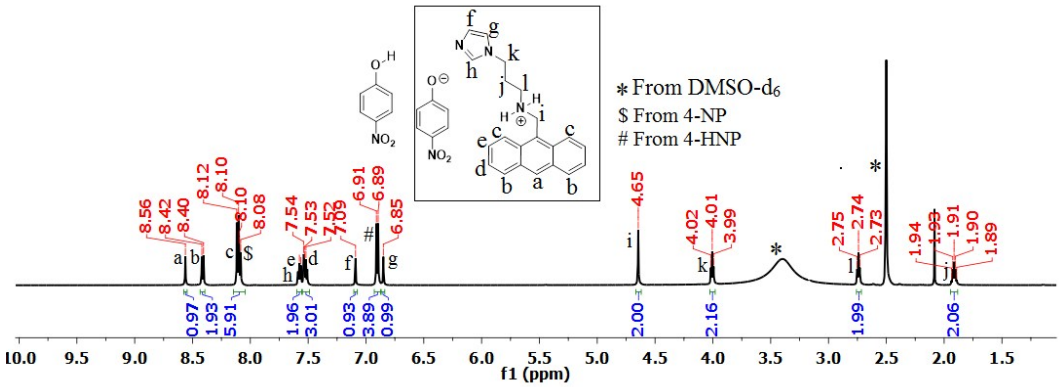


Figure S6: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of salt **H_2L.4-NP.4-HNP**.

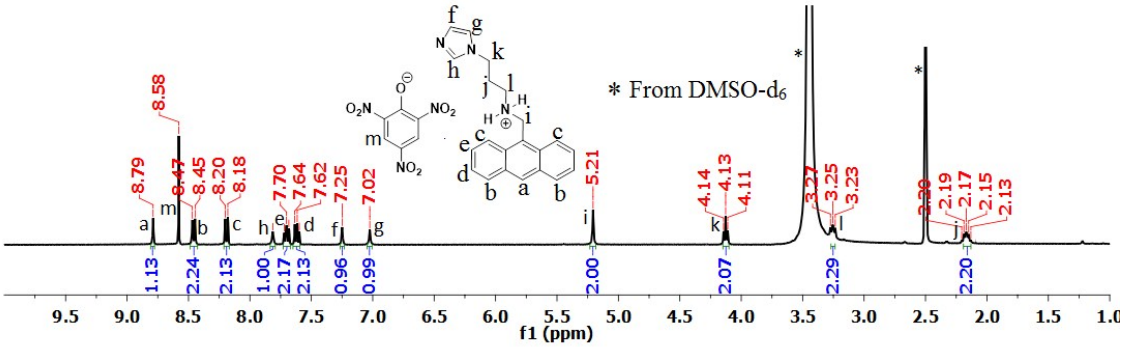


Figure S7: ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of salt **H_2L.2,4,6-TNP**.

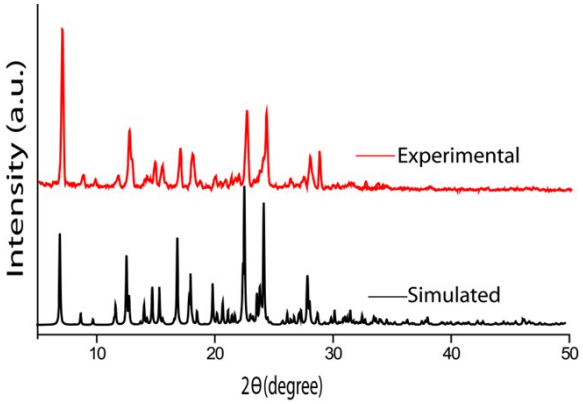


Figure S8: PXRD pattern of salt **H_2L.2-NBA** (Red = Experimental, Black = Simulated). Simulated pattern generated from CIF file.

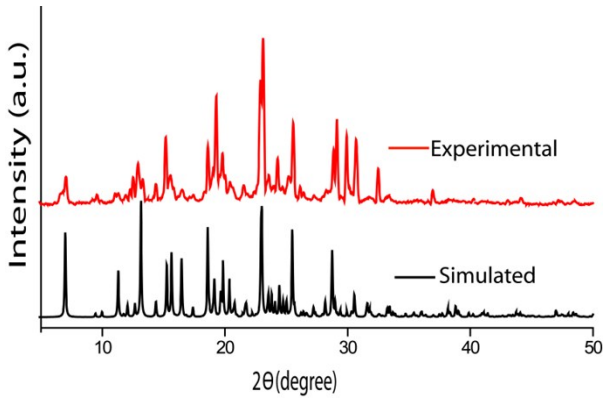


Figure S9: PXRD pattern of salt **H_2L.2,3-H_2DHBA** (Red = Experimental, Black= Simulated). Simulated pattern generated from CIF file.

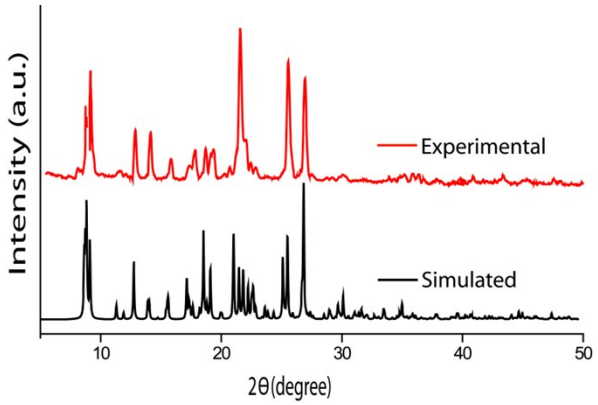


Figure S10: PXRD pattern of salt **H_2L.2,4-DNP** (Red = Experimental, Black = Simulated). Simulated pattern generated from CIF file.

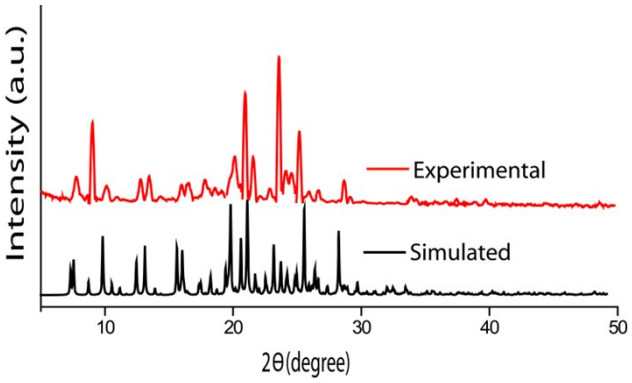


Figure S11: PXRD pattern of ionic cocrystal **H_2L.4-NP.4-HNP** (Red = Experimental, Black = Simulated). Simulated pattern generated from CIF file.

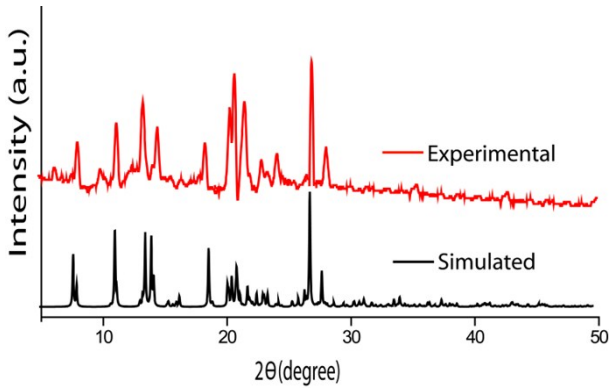
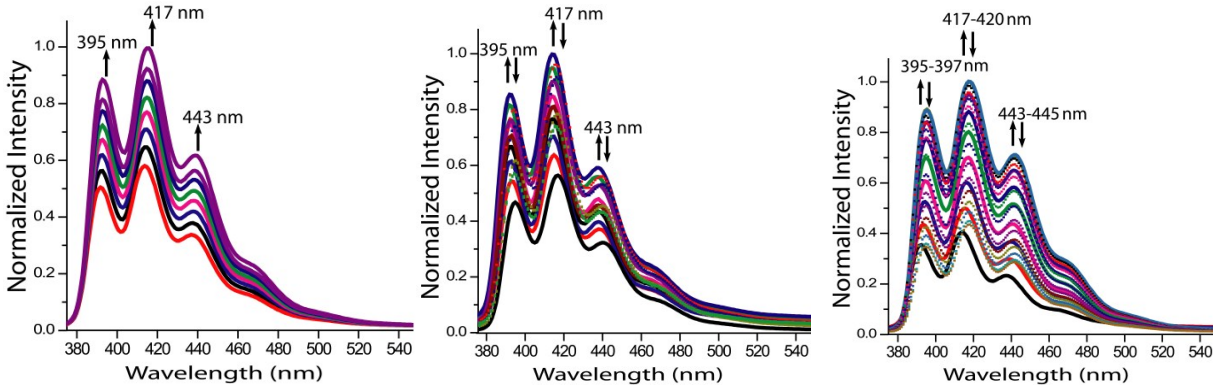
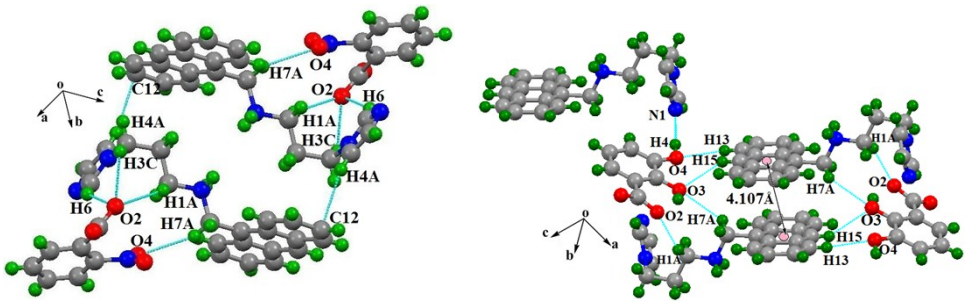


Figure S12: PXRD pattern of salt **H_2L.2,4,6-TNP** (Red = Experimental, Black = Simulated). Simulated pattern generated from CIF file.



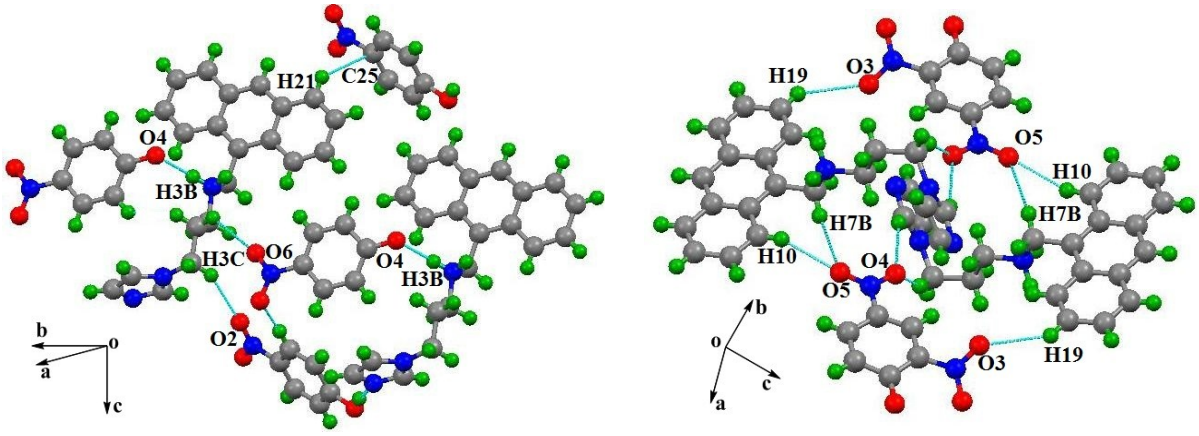
(a) (b) (c)

Figure S13: Fluorescence titration (excitation at 365 nm) of ligand **HL** (10^{-5} M in Ethanol) with (a) **2,3-H_3DHBA**, (b) **4-HNP** and (c) **2,4-HDNP** (10 µl aliquot of 10^{-5} M in Ethanol).showing enhancement (thick line) followed by quenching of emission (dashed line).

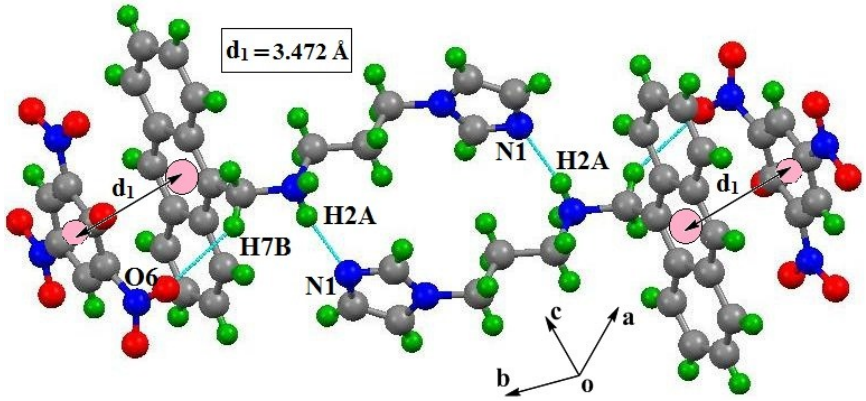


(a) (b)

Figure S14: Different types of hydrogen bonds present in salt (a) **H_2L.2-NBA** and (b) **H_2L.2,3-H_2DHBA**. O4-H4···N1 ($d_{D\cdots A}$ = 2.743Å, and $d_{H\cdots A}$= 1.935 Å) and C13-H13···O4 ($d_{D\cdots A}$ = 3.537 Å, and $d_{H\cdots A}$= 2.679 Å), C15-H15···O3 ($d_{D\cdots A}$ = 3.502, and $d_{H\cdots A}$= 2.713Å), C7-H7A···O3 ($d_{D\cdots A}$ = 3.398, and $d_{H\cdots A}$= 2.707Å) and C1-H1A···O2 ($d_{D\cdots A}$ = 3.580, and $d_{H\cdots A}$= 2.692Å).



(a) (b)



(c)

Figure S15: Different types of hydrogen bonds present in (a) ionic cocrystal **H_2L.4-NP.4-HNP**, (b) salt **H_2L.2,4-DNP** and (c) **H_2L.2,4,6-TNP**.

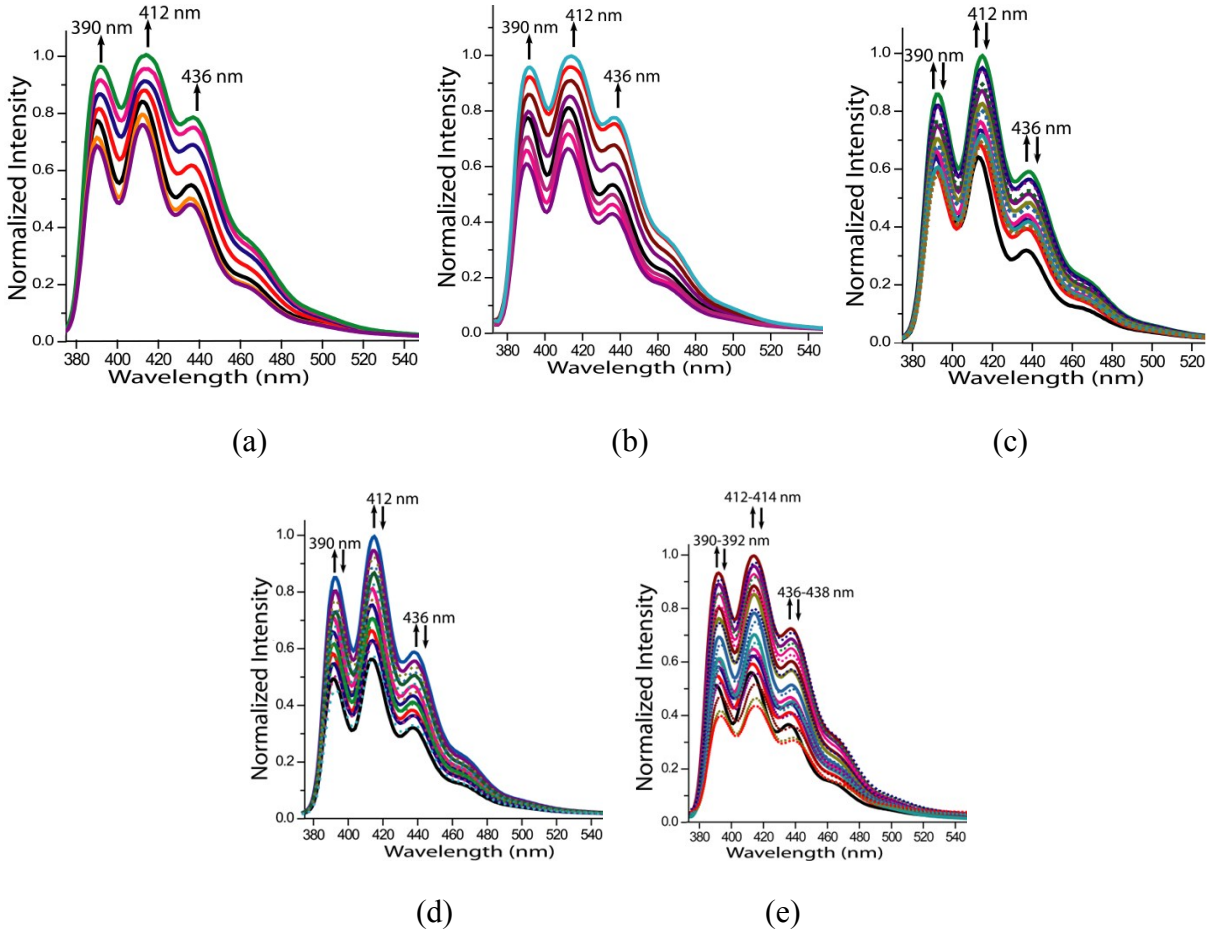
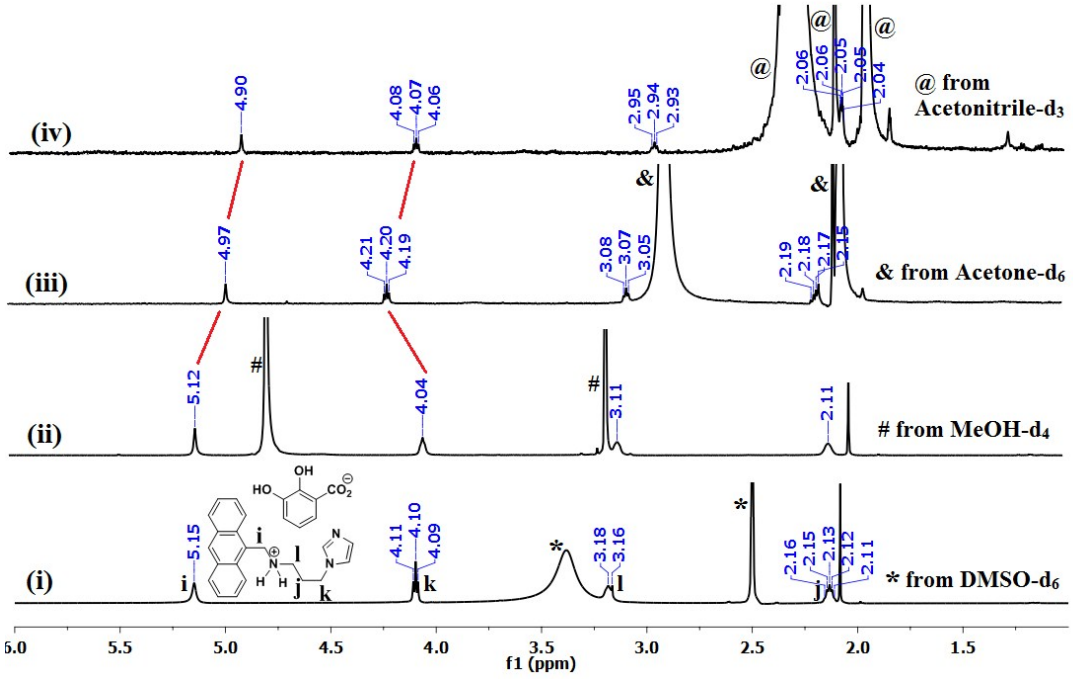
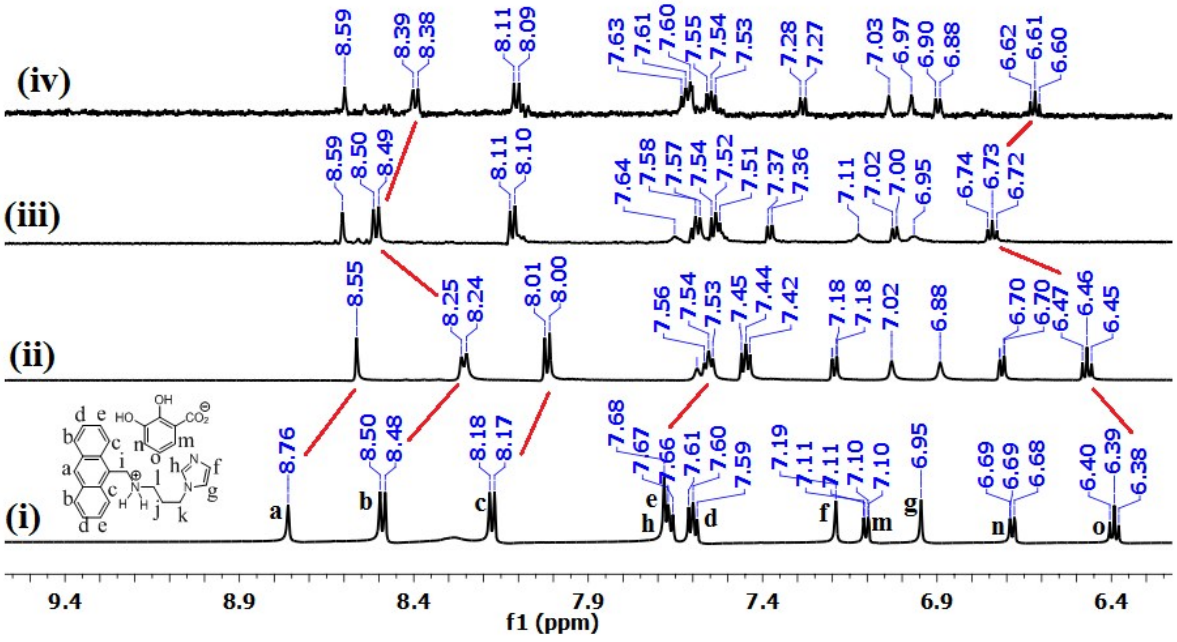


Figure S16: Fluorescence titration (excitation at 365 nm) of **HL** (10^{-5} M in Acetonitrile) with (a) **2-HNBA**, (b) **2,3-H_3DHBA**, (c) **4-HNP**, (d) **2,4-HDNP** and (e) **2,4,6-HTNP** (10 µL aliquot of 10^{-5} M in Ethanol) showing enhancement (thick line) followed by quenching of emission (dashed line).

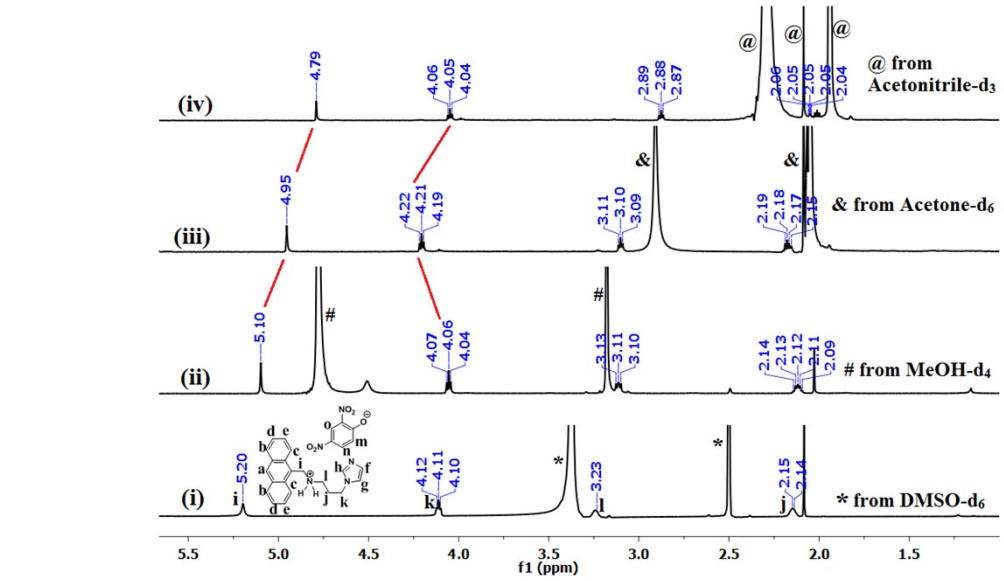


(a)

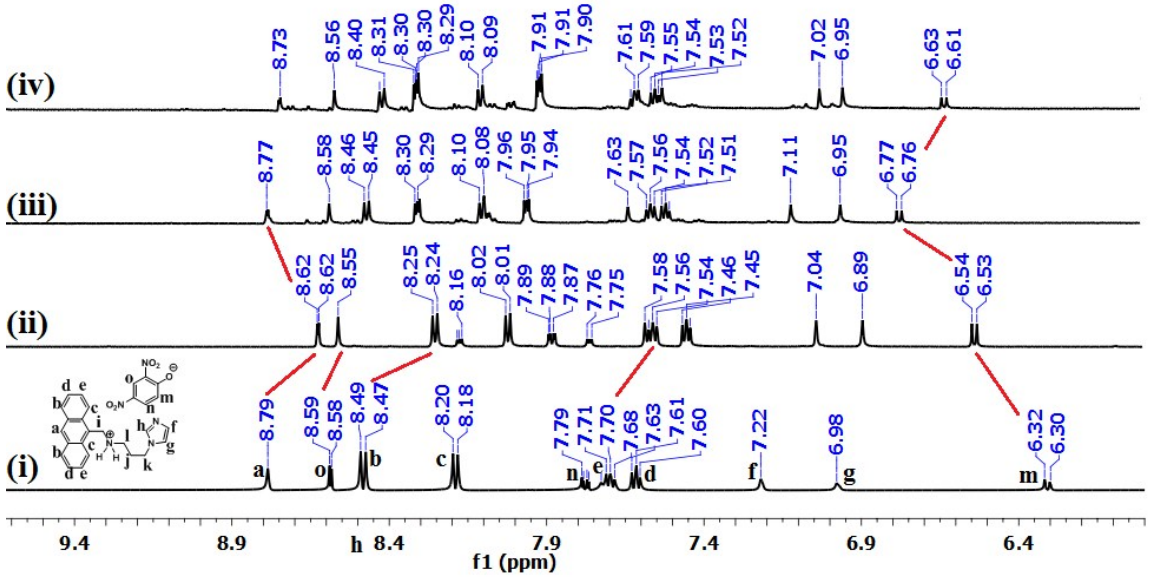


(b)

Figure S17: Solvent-dependent ^{1}H NMR spectra of **H_2L.2,3-H_2DHBA** in (i) DMSO-d_6, (ii) methanol-d_4 (iii) acetone-d_6 and (iv) acetonitrile-d_3. In (a) from 1-6ppm and (b) from 6-9.5ppm.

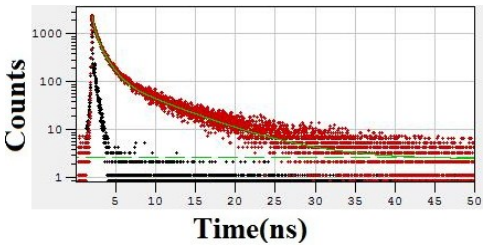


(a)



(b)

Figure S18: Solvent-dependent ^{1}H NMR spectra of **H_2L.2,4-DNP** in (i) DMSO-d_6, (ii) methanol-d_4 (iii) acetone-d_6 and (iv) acetonitrile-d_3. In (a) from 1-6ppm and (b) from 6-9.5ppm. (In acetonitrile and acetone compound is very less soluble hence there are peaks from decomposed part)



Exponential Components Analysis (Tail Fitting)

Fitting range : [148; 4096] channels

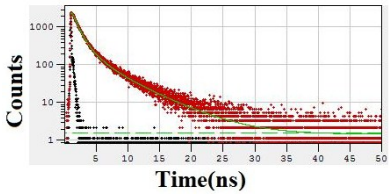
χ^2 : 1.318

	B_i	ΔB_i	f_i (%)	Δf_i (%)	τ_i (ns)	$\Delta\tau_i$ (ns)
1	1250.0144	23.7158	14.263	5.142	0.293	0.100
2	1115.1504	23.8301	49.495	1.616	1.141	0.013
3	142.8581	2.6750	36.242	0.689	6.520	0.002

Shift : 0 ns (± 0 ns)

Decay Background : 2.467 (± 0.077)

Figure S19: Time resolved fluorescence emission of solid sample of **HL** (λ_{ex} = 365 nm, λ_{em} = 446 nm).



Exponential Components Analysis (Reconvolution)

Fitting range : [66; 4096] channels

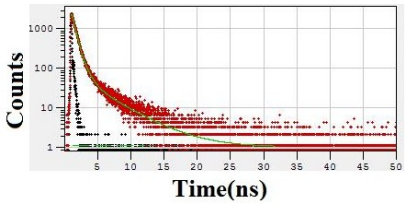
χ^2 : 1.079

	B_i	ΔB_i	f_i (%)	Δf_i (%)	τ_i (ns)	$\Delta\tau_i$ (ns)
1	0.0680	0.0025	40.328	3.286	0.752	0.034
2	0.0236	0.0024	33.354	3.910	1.789	0.031
3	0.0062	0.0004	26.318	1.668	5.347	0.004

Shift : -0.010 ns (± 0.179 ns)

Decay Background : 1.436 (± 0.062)

Figure S20: Time resolved fluorescence emission of solid sample of **H_2L.2-NBA** (λ_{ex} = 365 nm, λ_{em} = 544 nm).



Exponential Components Analysis (Reconvolution)

Fitting range : [64; 2600] channels

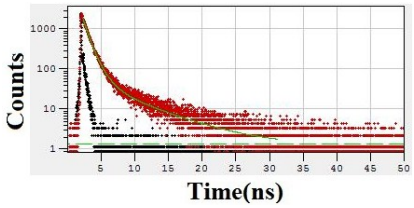
χ^2 : 1.013

	B_i	ΔB_i	f_i (%)	Δf_i (%)	τ_i (ns)	$\Delta\tau_i$ (ns)
1	0.0828	0.0029	52.223	10.543	0.405	0.067
2	0.0240	0.0031	33.984	6.491	0.907	0.055
3	0.0020	0.0001	13.793	0.844	4.344	0.007

Shift : -0.027 ns (± 0.178 ns)

Decay Background : 1.044 (± 0.082)

Figure S21: Time resolved fluorescence emission of solid sample of **H_2L.2,3-H_2DHBA** (λ_{ex} = 365 nm, λ_{em} = 494 nm).



Exponential Components Analysis (Tail Fitting)

Fitting range : [168; 2550] channels

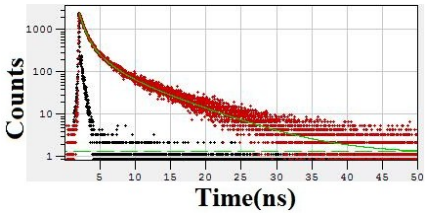
χ^2 : 1.175

	B_i	ΔB_i	f_i (%)	Δf_i (%)	τ_i (ns)	$\Delta\tau_i$ (ns)
1	1423.2976	150.3875	51.203	9.810	0.717	0.062
2	474.2506	149.8146	32.542	12.132	1.368	0.078
3	50.8017	5.6178	16.254	1.825	6.381	0.011

Shift : 0 ns (± 0 ns)

Decay Background : 1.228 (± 0.224)

Figure S22: Time resolved fluorescence emission of solid sample of **H_2L.4-NP.4-HNP** (λ_{ex} = 365 nm, λ_{em} = 413 nm).



Exponential Components Analysis (Tail Fitting)

Fitting range : [150; 4096] channels

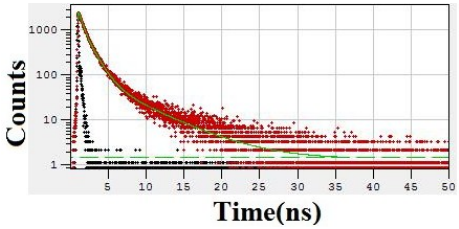
χ^2 : 1.086

	B_i	ΔB_i	f_i (%)	Δf_i (%)	τ_i (ns)	$\Delta\tau_i$ (ns)
1	1773.9342	29.1697	32.356	1.920	0.634	0.027
2	575.8865	27.1244	32.885	1.865	1.984	0.019
3	174.8727	7.2059	34.759	1.446	6.905	0.003

Shift : 0 ns (± 0 ns)

Decay Background : 1.203 (± 0.088)

Figure S23: Time resolved fluorescence emission of solid sample of **H_2L.2,4-DNP** (λ_{ex} = 365 nm, λ_{em} = 413 nm).



Exponential Components Analysis (Reconvolution)

Fitting range : [62; 3000] channels

χ^2 : 1.106

	B_i	ΔB_i	f_i (%)	Δf_i (%)	τ_i (ns)	$\Delta\tau_i$ (ns)
1	0.0589	0.0009	20.893	5.141	0.340	0.079
2	0.0484	0.0009	61.685	1.722	1.221	0.011
3	0.0031	0.0001	17.422	0.771	5.324	0.004

Shift : -0.003 ns (± 0.080 ns)

Decay Background : 1.357 (± 0.094)

Figure S24: Time resolved fluorescence emission of solid sample of **H_2L.2,4,6-TNP** (λ_{ex} = 365 nm, λ_{em} = 413 nm).

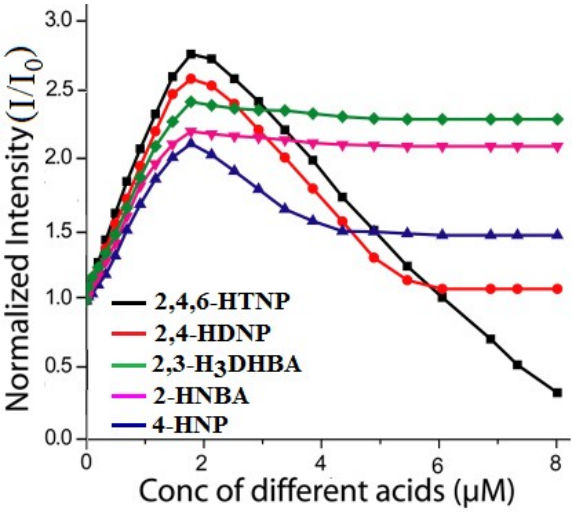


Figure S25: The changes in the normalised fluorescence intensities at 417 nm of **HL** (10^{-5} M) at different concentrations of carboxylic acids and nitrophenols.

DFT calculations details:

Gaussian 09 was used for all calculations. Optimization was done by DFT using B3LYP/6 functional using 31+G (d,p) as basis set.

Table S3: XYZ coordinates of **HL** :

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	6.143100	7.259600	3.740200
2	7	8.447800	6.887300	-0.008100
3	6	3.734200	8.931300	5.281900
4	6	6.710300	6.723800	2.468500
5	1	6.364900	7.234200	1.719800
6	1	6.433400	5.801000	2.356200
7	6	4.054600	7.570000	5.100900
8	6	4.648000	7.121800	3.791800
9	1	4.412800	6.192900	3.642000
10	1	4.259500	7.645700	3.074500
11	6	8.230500	6.796900	2.470500
12	1	8.571800	6.328600	3.248500
13	1	8.505200	7.724400	2.535300
14	6	3.131900	9.347300	6.522300

15	6	3.183800	7.059400	7.332600
16	6	8.830100	6.183400	1.213000
17	1	9.796700	6.187700	1.289900
18	1	8.544500	5.258300	1.146200
19	6	3.803500	6.626200	6.119600
20	6	3.978500	9.935100	4.300600
21	1	4.354000	9.691500	3.486200
22	6	2.860500	8.397000	7.498500
23	1	2.450400	8.667400	8.288600
24	6	4.107300	5.232400	5.999200
25	1	4.516100	4.918700	5.225300
26	7	7.313400	7.361800	-1.846300
27	6	2.886600	6.101300	8.350400
28	1	2.478300	6.381600	9.137400
29	6	2.829300	10.729900	6.709400
30	1	2.438200	11.007900	7.505600
31	6	7.459200	6.529700	-0.855900
32	1	6.937000	5.768800	-0.743600
33	6	3.101100	11.643400	5.753400
34	1	2.909600	12.540800	5.904100
35	6	3.672000	11.248100	4.529300
36	1	3.841700	11.882700	3.870700
37	6	3.808800	4.360300	6.996700
38	1	4.015900	3.458800	6.892500
39	6	3.191600	4.797400	8.185500
40	1	2.992900	4.185400	8.857200
41	6	8.961600	8.048800	-0.494700
42	1	9.661900	8.542800	-0.130500
43	6	8.259600	8.346200	-1.606500
44	1	8.391200	9.100000	-2.134600
45	1	6.693053	7.662741	4.471657

Table S4: XYZ coordinates of **H_2L.4NP** :

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.601879	-0.402567	1.380372
2	6	1.711326	-1.020128	1.034969
3	7	5.292692	-3.090364	0.019895
4	8	5.857818	-2.801543	-1.046823
5	6	2.422821	-0.717226	-0.160038
6	1	2.045357	0.061211	-0.817579
7	6	2.238179	-2.030736	1.881706

8	1	1.698805	-2.265187	2.793970
9	6	4.079698	-2.386899	0.364457
10	8	5.698056	-3.975952	0.788036
11	6	3.587181	-1.391091	-0.490410
12	1	4.128419	-1.160134	-1.400531
13	6	3.401408	-2.703053	1.552385
14	1	3.801409	-3.476096	2.197995
15	7	-0.862067	1.306206	0.329897
16	1	-1.542984	1.422402	1.080796
17	7	2.345431	4.291950	0.109649
18	7	3.246048	4.728254	-1.886923
19	6	-0.127861	2.583787	0.131747
20	1	-0.835952	3.364950	-0.179354
21	1	0.574433	2.428759	-0.693101
22	6	0.618470	3.008203	1.397142
23	1	1.295602	2.208829	1.712138
24	1	-0.094406	3.157657	2.218892
25	6	1.394079	4.323034	1.215263
26	1	0.703596	5.149315	1.017728
27	1	1.927688	4.561375	2.141517
28	6	-1.596604	0.862211	-0.904224
29	1	-0.853032	0.445954	-1.585157
30	1	-2.009811	1.747311	-1.398317
31	6	-2.697197	-0.127200	-0.595254
32	6	2.261589	5.006672	-1.057425
33	1	1.467828	5.721003	-1.232471
34	6	3.474401	3.500166	0.000401
35	1	3.784540	2.826759	0.785144
36	6	-2.480480	-1.521233	-0.734320
37	6	-3.957993	0.363540	-0.166604
38	6	4.009785	3.786483	-1.234295
39	1	4.902756	3.373654	-1.681804
40	6	-1.226844	-2.092066	-1.130516
41	1	-0.370132	-1.454254	-1.307587
42	6	-5.027535	-0.567661	0.116991
43	6	-3.567110	-2.438817	-0.463174
44	6	-4.803837	-1.938268	-0.046642
45	1	-5.613727	-2.634162	0.159586
46	6	-3.359399	-3.846275	-0.619323
47	1	-4.191595	-4.514530	-0.414927
48	6	-4.243493	1.758361	0.016711
49	1	-3.480519	2.500834	-0.190624
50	6	-1.065217	-3.448077	-1.263590
51	1	-0.097109	-3.844755	-1.553793
52	6	-2.144626	-4.342148	-1.011674

53	1	-1.995976	-5.411546	-1.125118
54	6	-5.474355	2.193358	0.443929
55	1	-5.654710	3.257223	0.568500
56	6	-6.296246	-0.074381	0.557270
57	1	-7.084175	-0.794345	0.761669
58	6	-6.519491	1.267821	0.721162
59	1	-7.486106	1.629653	1.057568
60	1	-0.100836	0.436039	0.764695

Table S5: XYZ coordinates of **H_2L.2,4,-DNP**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.452966	-0.353898	1.300545
2	8	-0.308017	-2.895505	2.331610
3	8	-1.056396	-4.302022	0.869995
4	7	-1.042416	-3.184551	1.385551
5	7	-5.352004	-2.183985	-0.568150
6	8	-5.672095	-3.363146	-0.367628
7	8	-6.086129	-1.403066	-1.159965
8	6	-1.566948	-0.801430	0.864059
9	6	-1.954570	-2.185580	0.868207
10	6	-3.167676	-2.637998	0.394047
11	1	-3.371887	-3.544857	0.406419
12	6	-4.068343	-1.728357	-0.096085
13	6	-2.546024	0.055125	0.292479
14	1	-2.346430	0.960313	0.227437
15	6	-3.760849	-0.366178	-0.164743
16	1	-4.371584	0.241585	-0.516437
17	7	1.148103	1.716854	0.370984
18	7	-2.499418	4.203567	0.262103
19	6	2.609976	-0.998553	-0.838856
20	6	0.215634	2.862755	0.162582
21	1	-0.409984	2.646078	-0.545948
22	1	0.721510	3.643562	-0.111777
23	6	2.992245	0.344385	-0.641516
24	6	1.976989	1.436384	-0.850188
25	1	2.438515	2.248862	-1.109974
26	1	1.388349	1.183808	-1.577945
27	6	-0.554817	3.183355	1.435365
28	1	0.073332	3.349989	2.155599
29	1	-1.096336	2.417902	1.681849
30	6	3.595599	-2.035830	-0.674492

31	6	5.280772	-0.371442	-0.141792
32	6	-1.454534	4.39915	1.263441
33	1	-1.868932	4.607883	2.114883
34	1	-0.910364	5.160595	1.006688
35	6	4.315014	0.673683	-0.276270
36	6	1.288121	-1.397578	-1.190601
37	1	0.636154	-0.747312	-1.315826
38	6	4.900610	-1.688115	-0.349322
39	1	5.538570	-2.360252	-0.266892
40	6	4.765165	2.015197	-0.059079
41	1	4.160830	2.717892	-0.132867
42	7	-3.514431	4.277137	-1.701396
43	6	6.632231	-0.040989	0.184644
44	1	7.262213	-0.719987	0.266687
45	6	3.198671	-3.395378	-0.854029
46	1	3.828117	-4.071890	-0.752511
47	6	-2.459166	4.621621	-1.021479
48	1	-1.751373	5.104698	-1.381950
49	6	1.926166	-3.719451	-1.167082
50	1	1.687347	-4.612968	-1.263527
51	6	0.957384	-2.715020	-1.349267
52	1	0.086643	-2.947320	-1.579736
53	6	6.060322	2.278973	0.253427
54	1	6.327277	3.160429	0.388411
55	6	7.005429	1.241278	0.376705
56	1	7.888600	1.441032	0.589577
57	6	-3.670928	3.527124	0.402967
58	1	-3.988803	3.120921	1.178243
59	6	-4.282261	3.558535	-0.798130
60	1	-5.098582	3.157812	-0.991688
61	1	1.772760	1.882400	1.157826
62	1	-0.575234	0.002763	2.183406

Table S6: XYZ coordinates of **H_2L.2,4,6-TNP**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.180928	-0.531399	0.109550
2	8	1.297422	-2.493546	-1.713266
3	8	3.154293	-2.462388	-2.801453
4	7	2.487515	-2.198285	-1.812344
5	8	3.191911	0.577170	3.521341
6	7	2.506467	0.144727	2.599248

7	8	1.283755	0.198769	2.666220
8	8	7.188504	-1.983341	-0.345432
9	6	3.150544	-1.570127	-0.669824
10	6	3.144726	-0.450957	1.458627
11	8	7.183600	-1.028484	1.616917
12	6	2.370696	-0.842365	0.294874
13	6	4.509415	-1.729667	-0.611472
14	1	4.972900	-2.155235	-1.296906
15	7	6.619421	-1.437312	0.592108
16	6	4.513855	-0.635187	1.539940
17	1	4.981374	-0.352472	2.291823
18	6	5.169537	-1.237049	0.501241
19	7	-1.089294	0.584122	1.031229
20	1	-1.394251	1.085411	1.699617
21	7	-0.061097	4.628883	-1.574649
22	7	0.549739	6.683698	-1.018409
23	6	-3.001275	-1.025909	0.566860
24	6	-1.648252	-0.811979	1.204042
25	1	-1.021645	-1.445949	0.822771
26	1	-1.718644	-1.002263	2.152993
27	6	-3.081672	-1.642433	-0.704764
28	6	-4.166795	-0.675584	1.278447
29	6	-0.619246	2.605229	-0.307570
30	1	-0.878093	3.154253	0.448325
31	1	0.329232	2.416678	-0.222406
32	6	-1.385850	1.295149	-0.247341
33	1	-2.337463	1.471297	-0.308691
34	1	-1.133252	0.734242	-0.997891
35	6	-0.847685	3.388489	-1.579656
36	1	-0.593433	2.846370	-2.343084
37	1	-1.789793	3.601828	-1.662452
38	6	-5.454468	-0.934822	0.667128
39	6	-4.370186	-1.922004	-1.285737
40	6	-0.424590	5.781251	-1.051700
41	1	-1.282541	5.947877	-0.734751
42	6	1.606267	6.015175	-1.564129
43	1	2.455035	6.379242	-1.674570
44	6	-1.938070	-1.995094	-1.476228
45	1	-1.088500	-1.812453	-1.145767
46	6	-4.152380	-0.088544	2.562391
47	1	-3.338966	0.109242	2.964908
48	6	-5.502850	-1.542799	-0.570455
49	1	-6.338480	-1.707580	-0.947271
50	6	1.265861	4.760725	-1.922411
51	1	1.811583	4.120934	-2.320183

52	6	-4.434508	-2.562896	-2.552318
53	1	-5.263206	-2.762641	-2.922975
54	6	-6.627320	-0.610158	1.392223
55	1	-7.458777	-0.772733	1.009109
56	6	-2.068276	-2.584813	-2.673381
57	1	-1.304723	-2.801535	-3.154893
58	6	-5.320670	0.195021	3.228436
59	1	-5.293442	0.563212	4.081627
60	6	-3.318301	-2.883581	-3.218882
61	1	-3.375702	-3.305714	-4.046011
62	6	-6.564590	-0.076344	2.612090
63	1	-7.353072	0.121753	3.064861
64	1	0.657799	-0.801195	0.867933

Table S7: XYZ coordinates of **H_2L.2-NBA**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-5.581076	-0.915570	-0.797355
2	1	-6.032664	-0.110996	-0.915339
3	7	-0.108987	-2.191334	0.330363
4	1	0.264642	-2.571331	1.043895
5	7	-4.458020	-2.524838	0.111497
6	6	1.917535	-0.121987	-1.227615
7	6	2.017459	-1.448917	-0.754312
8	6	3.070707	0.728631	-1.179154
9	6	0.808120	-2.344124	-0.842757
10	1	0.320147	-2.137767	-1.655489
11	1	1.100591	-3.267142	-0.898446
12	6	3.238333	-1.934805	-0.243311
13	6	-1.444730	-2.808496	0.093200
14	1	-1.324714	-3.724744	-0.201306
15	1	-1.896951	-2.325489	-0.615931
16	6	4.382205	-1.068865	-0.210020
17	6	0.723082	0.435472	-1.772164
18	1	-0.043770	-0.088689	-1.816429
19	6	-2.309164	-2.794356	1.335091
20	1	-2.381583	-1.885188	1.665359
21	1	-1.888042	-3.329704	2.025195
22	6	4.262237	0.234798	-0.670281
23	1	5.003754	0.795219	-0.636240
24	6	-3.703006	-3.340581	1.054660
25	1	-3.624005	-4.239927	0.700350

26	1	-4.194873	-3.393390	1.889026
27	6	2.976224	2.059559	-1.683392
28	1	3.726089	2.609224	-1.666155
29	7	-5.429012	-1.858893	-1.758073
30	6	0.679366	1.708963	-2.224341
31	1	-0.116142	2.045176	-2.569441
32	6	1.818308	2.533551	-2.183545
33	1	1.771910	3.407023	-2.501346
34	6	3.410987	-3.266975	0.242690
35	1	2.684153	-3.848110	0.249642
36	6	5.625698	-1.576631	0.278270
37	1	6.370840	-1.020388	0.302947
38	6	-4.747376	-2.815808	-1.168112
39	1	-4.493385	-3.605575	-1.588737
40	6	-4.995771	-1.296244	0.340773
41	1	-4.961651	-0.815395	1.135869
42	6	5.733775	-2.853285	0.703831
43	1	6.552249	-3.173618	1.005684
44	6	4.612791	-3.700264	0.692012
45	1	4.696803	-4.573239	1.000032
46	8	-0.385258	0.063272	1.871841
47	8	-0.338668	1.904169	3.109105
48	8	1.452504	3.107477	1.254560
49	7	0.521823	3.860343	1.049969
50	8	0.564773	5.072946	1.264706
51	6	-0.555591	1.302530	2.050208
52	6	-1.161603	2.068624	0.903344
53	6	-0.718151	3.313869	0.487012
54	6	-2.303387	1.575981	0.285983
55	1	-2.630285	0.738565	0.524281
56	6	-1.353235	4.067165	-0.481618
57	1	-1.021813	4.897877	-0.736998
58	6	-2.489035	3.550696	-1.057260
59	1	-2.941909	4.040174	-1.706021
60	6	-2.960925	2.317369	-0.681483
61	1	-3.728803	1.976271	-1.080530
62	1	-0.960679	-0.240503	1.166001

Table S8: XYZ coordinates of **H_2L.2,3-H_2DHBA**:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	1.314656	-0.234570	1.079980

2	8	3.919897	-2.712239	-0.874787
3	1	3.106477	-2.643205	-0.944402
4	8	6.520346	-2.656877	-0.412523
5	1	7.241841	-2.700072	-0.024074
6	8	1.639212	-1.654168	-0.580441
7	6	3.553185	-0.762268	0.480765
8	6	4.393273	-1.707086	-0.099049
9	6	2.077747	-0.896531	0.317989
10	6	4.102454	0.261193	1.257639
11	1	3.546789	0.893855	1.652163
12	6	5.772013	-1.660343	0.131822
13	6	6.293529	-0.627622	0.879003
14	1	7.211974	-0.571916	1.010853
15	6	5.457966	0.334174	1.439060
16	1	5.821032	1.029901	1.937845
17	7	-1.206674	-0.469173	0.072030
18	1	-1.733227	-0.229433	0.747760
19	7	-3.252866	-4.264988	0.048387
20	7	-5.169598	-4.134418	-1.033398
21	6	-1.552608	-1.848253	-0.351447
22	1	-1.003743	-2.093802	-1.112718
23	1	-2.480638	-1.871069	-0.634274
24	6	-2.418576	2.565860	-0.064484
25	6	-1.261144	1.943467	-0.574795
26	6	-0.056276	2.653027	-0.688382
27	6	-1.359740	0.512959	-1.042362
28	1	-2.220790	0.377273	-1.467835
29	1	-0.671879	0.347966	-1.705482
30	6	-1.345432	-2.863131	0.758723
31	1	-1.837647	-2.585179	1.547736
32	1	-0.404462	-2.903612	0.989213
33	6	-0.013591	4.041455	-0.310661
34	6	-1.822496	-4.241431	0.321934
35	1	-1.340544	-4.506446	-0.477338
36	1	-1.620649	-4.884219	1.018870
37	6	-3.867399	-4.184044	-1.147120
38	1	-3.417495	-4.166224	-1.961369
39	6	-2.354489	3.953149	0.323747
40	6	-3.670651	1.902600	0.081653
41	1	-3.742359	1.009352	-0.164720
42	6	1.157769	2.079780	-1.174951
43	1	1.168201	1.184359	-1.424649
44	6	-1.158931	4.647760	0.182282
45	1	-1.126800	5.545520	0.424096
46	6	-4.243639	-4.256426	0.988353

47	1	-4.138035	-4.293544	1.911911
48	6	1.208048	4.767648	-0.470495
49	1	1.236466	5.668299	-0.242578
50	6	-4.761880	2.545085	0.571398
51	1	-5.566974	2.086337	0.660455
52	6	-3.531615	4.588574	0.819389
53	1	-3.502087	5.487372	1.057318
54	6	2.315896	4.170718	-0.945812
55	1	3.098537	4.662712	-1.050252
56	6	-4.685163	3.906120	0.946682
57	1	-5.438824	4.332713	1.285765
58	6	-5.404546	-4.182251	0.308316
59	1	-6.248347	-4.166698	0.700291
60	6	2.296262	2.809638	-1.282489
61	1	3.076127	2.400753	-1.584102
62	1	0.518324	0.008957	0.602329
