Supplementary Data for Manuscript:

"Discovery of dual fluorescent 1,8-NI dyes based on balanced Seesaw photophysical model"

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General Experimental: In a typical reaction, 1 mmol of the 4-substituted naphthalic anhyride was combined with 1.1 mmol of the 4-substituted aminoarene. The reactants were refluxed in approximately 3-4 mL pyridine for a period of 12 hr. Pyridine was removed in the fume hood via stream of air and the residue was filtered using a plug of silica gel with the appropriate solvent as found through TLC analysis. Recrystallization was further carried out using ethanol.

General procedure for preparation of 4-cyano-1,8-naphthalic anhydride:

4-bromo-1,8-naphthalic anhydride (3.1mmole) and tetraethyl ammonium cyanide (7.0mmole), CuCN (11.0 mmole), $Pd_2(dba)_3$ (0.12mmole) (tris (dibenzylidene acetone) dipalladium), DPPF (0.48mmole) (1-Diphenylphosphino-1-(di-tert-butyl phosphino)-ferrocene were dissolved in 15 ml of anhydrous1,4-dioxane. The resulting mixture was refluxed in presence of argon gas for 3 hr. The reaction mixture was filtered over Celite-521 and the product was purified in 50:50 of ethyl acetate and hexane solution.

4-Cyano-*N*-(4'-methoxyphenyl)-1,8-naphthalimide (**1**) m.p. 180 ºC; ^{1}H NMR DMSO-d6 δ, 8.61 (dd, *J* = 7.7 Hz, 2H), 8.37 (d, *J* = 8.1 Hz, 1H), 8.35 (d, 8.0 Hz, 1H) 8.15 (dd, J_{app} = 7.5 Hz, 1H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 2H) 3.83 (s, 3H)

^{13}C DMSO-d6, δ 164.3, 159.5, 133.3, 132.3, 131.9, 131.7, 130.9, 130.6, 130.5, 129.8, 129.4, 128.7, 123.9, 114.8, 55.7.

IR cm^{-1} ν = 2361, 1707, 1513, 1364, 1238, 1187, 829, 789.

Anal. Calcd. for $C_{20}H_{12}N_2O_3$: C, 73.2; H, 3.66; N, 8.54. Found: C, 72.8; H, 3.74; N, 8.66

4-Sulfo- *N*-(4'-methoxyphenyl-1,8-naphthalimide (**2**) m.p. 288 ºC dec; ^{1}H NMR DMSO-d6, δ, 9.30 (d, *J* = 8.9 Hz, 1H), 8.47 (dd, *J* = 8.0 Hz, 2H), 8.26 (d, *J* = 6.9 Hz, 1H), 7.90 (dd, J_{app} = 7.4 Hz, 1H), 7.34 (d, *J* = 14 Hz, 2H), 7.09 (d, *J* = 14 Hz, 2H). 3.83 (s, 3H)

^{13}C NMR DMSO-d6 δ, 164.3, 164.1, 159.5, 134.9, 134.7, 131.1, 130.8, 130.7, 130.5, 129.1, 128.9, 127.2, 123.9, 123.2, 115.2, 114.8, 56.0.

IR cm^{-1} ν = 1658, 1514, 1243, 1262, 1196, 1070, 1032, 785, 754,

Anal. Calcd. for $C_{19}H_{13}NSO_6K \bullet 2H_2O$: C, 50.0; H, 2.8; N, 3.06 Found: C, 49.7; H, 2.9; N, 3.10

4-Chloro-*N*-(4'-methoxyphenyl)-1,8-naphthalimide (**3**) m.p. 215 ºC; ^{1}H DMSO-d6, δ 8.68 (d, *J* = 8.6 Hz, 1H), 8.42 (d, *J* = 7.1 Hz, 1H) 8.19 (d, *J* = 8.3 Hz, 1H), 7.69 (dd, J_{app} = 8.3 Hz, 1H), 7.21 (d, *J* = 8.5 Hz, 2H), 7.03, (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 7.7 Hz, 1H), 3.83 (s, 3H)

^{13}C DMSO-d6, δ 164.9, 163.9, 159.2, 153.3, 134.5, 131.6, 130.7, 129.7, 129.6, 124.5, 122.9, 121.2, 120.0, 114.5, 108.7, 108.5, 55.9.

IR cm^{-1} ν = 1650, 1513, 1240, 1022, 818, 790

Anal. Calcd. for $C_{19}H_{12}NO_3$: C, 75.4; H, 3.9; N, 4.64 Found: C, 75.3; H, 3.6; N, 4.78

4-Cyano-*N*-(4'-aminophenyl)-1,8-naphthalimide (**4**) m.p. 220 ºC; ^{1}H NMR DMSO-d6 δ, 8.54 (d, *J* = 8.0 Hz, 2H), 8.31 (d, *J* = 7.7 Hz, 1H), 8.20 (d, 7.7 Hz, 1H) 7.99 (dd, J_{app} = 8.0 Hz, 1H), 6.96 (d, *J* = 8.2 Hz, 2H), 6.65 (d, *J* = 8.5 Hz, 2H)

^{13}CDMSO-d6, d, 163.9, 149.1, 132.2, 131.9, 131.5, 130.5, 130.1, 129.8, 129.8, 129.7, 129.5, 129.4, 129.3, 129.3, 124.2, 124.1, 123.3.

IR cm^{-1} ν = 2359, 1709, 1654, 1514, 1374, 1237, 1168, 834, 783.

Anal. Calcd. for $C_{19}H_{11}N_3O_2$: C, 76.3; H, 3.68; N,13.4: Found: C, 76.7; H, 3.74, N, 13.2.

4-Sulfo-*N*-(4'-aminophenyl-1,8-naphthalimide (**5**) m.p. 270 ºC; ^{1}H DMSO-d6 δ 9.38 (d, *J* = 8.6 Hz, 1H) 8.51-8.45 (m, 2H), 8.27 (d, *J* = 7.4 Hz, 1H), 7.90 (t, *J* = 7.4, 1H), 7.44 (d, J_{app} = 8.8 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 2H)

^{13}C DMSO d-6 δ 164.3, 163.9, 151.2, 135.9, 135.2, 134.9, 133.8, 131.0, 130.9, 129.2, 128.4, 127.3, 125.5, 123.6, 123.0, 122.1

IR cm^{-1} ν = 1161, 1514, 1242, 1167, 1032, 751, 657.

Anal. Calcd. for $C_{18}H_{12}N_2SO_5$: C, 58.7; H, 3.26; N, 7.60. Found: C, 58.3; H, 3.03, N, 7.59

4-Chloro-*N*-(4'-aminophenyl)-1,8-naphthalimide (**6**) m.p. 235 ºC dec; ^{1}H DMSO -d6, δ 8.62 (d, *J* = 8.6 Hz, 1H), 8.57 (d, *J* = 8.0 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 8.10-8.00 (m, 2H), 6.99 (d, *J* = 8.5 Hz, 2H), 6.66 (d, *J* = 8.6 Hz, 2H), 5.25 (s, 2H)

^{13}C DMSO-d6 δ 164.1, 163.8, 149.2, 137.8, 132.1, 131.4, 130.5, 129.7, 129.2, 129.1, 129.0, 128.2, 124.1, 123.9, 122.7, 114.3.

IR cm^{-1} ν =1712, 1662, 1303, 1009, 771, 751.

Anal. Calcd. for $C_{18}H_{11}N_2O_2Cl$: C, 67.1; H, 3.42; N, 8.69 Found: C, 66.8; H, 3.38, N, 8.70

4-Cyano-*N*-(4'-thiophenyl)-1,8-naphthalimide (**7**) m.p. 200 ºC; ^{1}H NMR DMSO-d6 δ, 8.64 –8.56 (m, 4H), 8.13 (t, *J* = 7.5 Hz, 1H), 7.76 (d, 7.7 Hz, 2H) 7.48 (d, *J* = 8.0 Hz, 2H)

^{13}C DMSO-d6, δ 163.6, 163.2, 146.3, 136.5, 134.4, 132.4, 131.3, 131.1, 130.7, 130.6, 129.8, 128.0, 127.9, 116.7, 114.7.

IR cm^{-1} ν = 2360, 1677, 1648, 1561, 1345, 1228, 790, 738.

Anal. Calcd. for $C_{19}H_{10}N_2SO_2$: C, 69.1; H, 3.03; N, 8.48. Found: C, 68.9; H, 3.74; N, 8.42

4-Sulfo-*N*-(4'-thiophenyl)-1,8-naphthalimide (**8**) m.p. 230 ºC dec; ^{1}H DMSO-d6 δ 9.31 (d, *J* = 8.5 Hz, 1H), 8.49 (pseudo t, *J* = 7.8 Hz, 2H), 8.25 (d, *J* = 7.4 Hz, 1H) 7.91 (dd, J_{app} = 7.4 Hz, 1H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H)

^{13}C DMSO-d6, δ 164.4, 164.1, 150.6, 134.9, 134.7, 131.1, 130.8, 129.1, 128.9, 128.3, 127.4, 125.8, 125.5, 123.9, 123.2, 115.2.

IR cm^{-1}, ν = 1661, 1371, 1240, 1192, 1068, 1042, 783, 753.

Anal. Calcd. for $C_{18}H_{11}NS_2O_5$ K•3H_2O: C, 45.2; H, 2.32; N, 4.84. Found: C, 45.2; H, 2.24; N, 4.76.

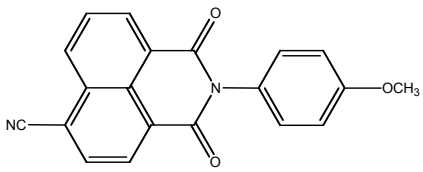
4-Chloro-*N*-(4'-thiophenyl)-1,8-naphthalimide (**9**) m.p. 226 ºC dec; ^{1}H DMSO-d6 δ 8.64 (d, *J*= 8.2 Hz, 1H), 8.42 (d, *J* = 7.4 Hz, 1H), 8.18 (d, *J*=7.9 Hz, 1H), 7.67 (dd, J_{app} = 8.5 Hz, 1H), 7.46 (s, 2H), 7.18 (d, *J*= 7.5Hz, 2H), 7.03 (d, *J* = 9.1 Hz, 2H), 6.87 (d, *J* = 8.6 Hz, 1H).

^{13}C NMR DMSO-d6 δ, 164.0, 163.9, 137.4, 132.9, 131.6, 131.3, 131.1, 130.9, 130.5, 130.3, 129.6, 128.3, 128.2, 124.4, 124.1, 115.7

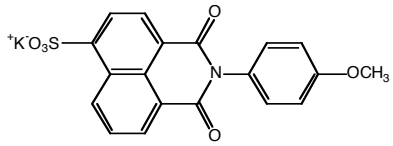
IR cm^{-1}, v = 1656, 1583, 1512, 1365, 1238, 1173, 818, 789.

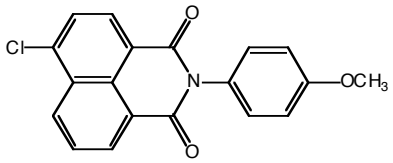
Anal. Calcd. for $C_{18}H_{10}NSO_2Cl$: C, 63.7; H, 3.11; N, 4.13 Found: C, 63.4; H, 3.03; N, 4.10.

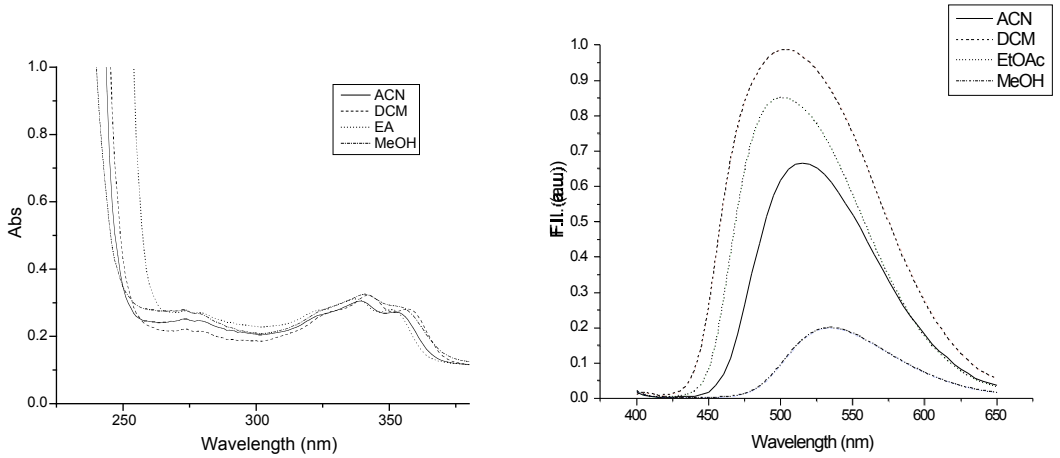
Appendix I Photophysical properties of 4-substituted-*N*-(4'-phenyl)-1,8-naphthalimides

 (**1**) 4-Cyano-*N*-(4'-methoxy phenyl)-1,8-NI	Absorbance λmax, (ε)	λex (nm)	λem (nm)	F.Intensity (a.u.)	Quantum Yield*
DCM M = 1.0 x 10^{-5}	342(0.193) 410(0.126)	410	521 603	1.8 x 10^{7} 1.8 x 10^{7}	4.6 x10^{-2} 4.6 x10^{-2}
ACN M = 1.0 x 10^{-5}	340(0.191) 410(0.126)	410	571	1.8 x 10^{7}	4.6 x10^{-2}
EtOAc M = 1.0 x 10^{-5}	338(0.200) 410(0.128)	410	527 601	1.8 x 10^{7} 1.8 x 10^{7}	4.5 x10^{-2} 4.5 x10^{-2}
MeOH M = 1.0 x 10^{-5}	340(0.153) 410(0.120)	410	588	1.6 x 10^{7}	4.3 x10^{-2}
Acetone M = 1.0 x 10^{-5}	339(0.195) 410(0.125)	410	541 600	1.8 x 10^{7} 1.8 x 10^{7}	4.6 x10^{-2} 4.6 x10^{-2}

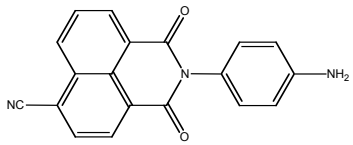
*Quantum yields relative to Quinine sulfate standard

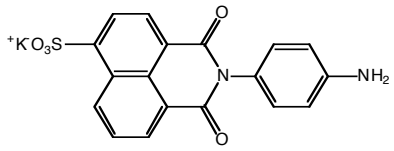
 **(2)** 4-Sulfo -*N* (4-methoxy phenyl) NI	λmax (Abs)	λex (nm)	λem (nm)	F.Intensity A.U.	Quantum yield
Dichloromethane M = 1.0 x 10^{-5}	338 (0.233)	340	369 512	2.62x10^{5} 2.09x10^{5}	3.6 x10^{-4} 2.8 x10^{-4}
Ethyl Acetate M = 1.0 x 10^{-5}	338 (0.246)	340	360 530	2.10 x10^{5} 2.16 x10^{5}	2.7 x10^{-4} 2.8 x10^{-4}
Acetonitrile M = 1.0 x 10^{-5}	341 (0.242)	340	364 562	2.92 x10^{5} 1.02x10^{5}	3.8 x10^{-4} 1.3 x10^{-4}
MeOH M = 1.0 x 10^{-5}	339 (0.256)	340	368	1.53 x10^{5}	1.9 x10^{-4}

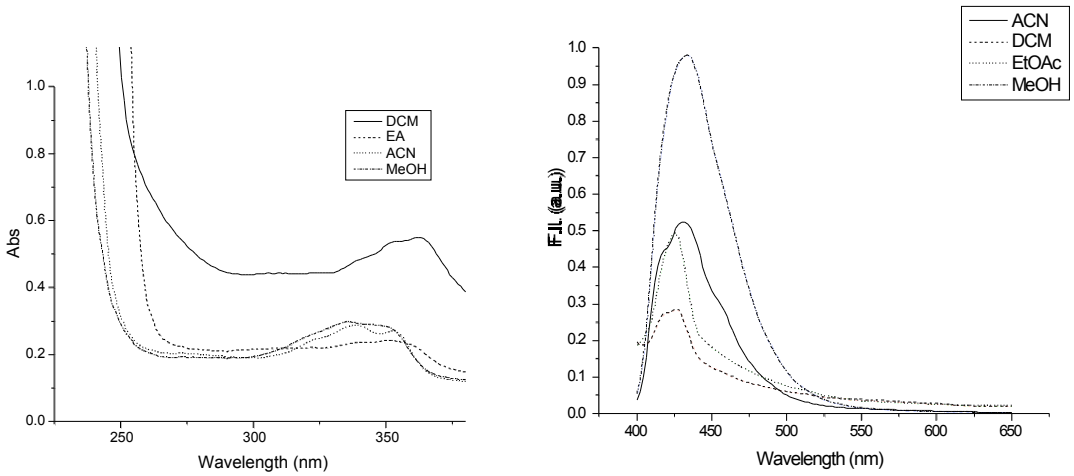
 (**3**) 4-Chloro-*N*-(4'-methoxy) phenyl NI	λmax (Abs)	λex (nm)	λem (nm)	F.Intensity A.U.	Quantum yield
Dichloromethane M = 1.0 x 10^{-5}	340 (0.305)	410	505	7.35 x10^{6}	7.7 x10^{-3}
Ethyl Acetate M = 1.0 x 10^{-5}	342 (0.300)	410	494	7.21x10^{6}	7.6 x10^{-3}
Acetonitrile M = 1.0 x 10^{-5}	338 (0.312)	410	516	6.21 x10^{6}	6.4 x10^{-3}
Methanol M = 1.0 x 10^{-5}	341 (0.324)	410	536	2.87 x10^{6}	2.8 x10^{-3}



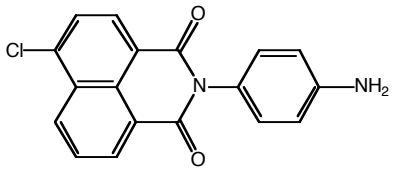
Supplementary Figure 1. Absorption and fluorescence spectra of (**3**) 4-Chloro-*N*-(4'-methoxyphenyl)-1,8-NI.

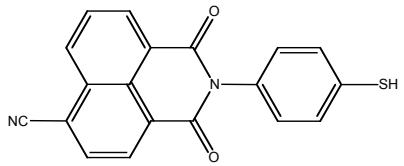
 (**4**) 4-Cyano-*N*-(4'-amino phenyl)-1,8-NI	Absorbance	λex (nm)	λem (nm)	F.Intensity (a.u.)	Quantum yield
DCM M = 1.0 x 10^{-5}	339(0.562) 420(0.134)	420	520 576	5.4 x10^{6} 6.0 x 10^{6}	1.3 x10^{-2} 1.4 x10^{-2}
ACN M = 1.0 x 10^{-5}	336(0.374) 420(0.126)	420	515 581	2.0 x 10^{6} 1.0 x 10^{7}	5.1 x10^{-3} 2.5 x 10^{-2}
EtOAc M = 1.0 x 10^{-5}	334(0.573) 420(0.141)	420	511 575	1.9 x 10^{6} 6.5 x 10^{6}	4.3 x10^{-3} 1.5 x10^{-2}
MeOH M = 1.0 x 10^{-5}	337(0.562) 420(0.142)	420	522 579	1.7 x 10^{6} 4.0 x 10^{6}	3.8 x10^{-3} 9.0 x10^{-3}

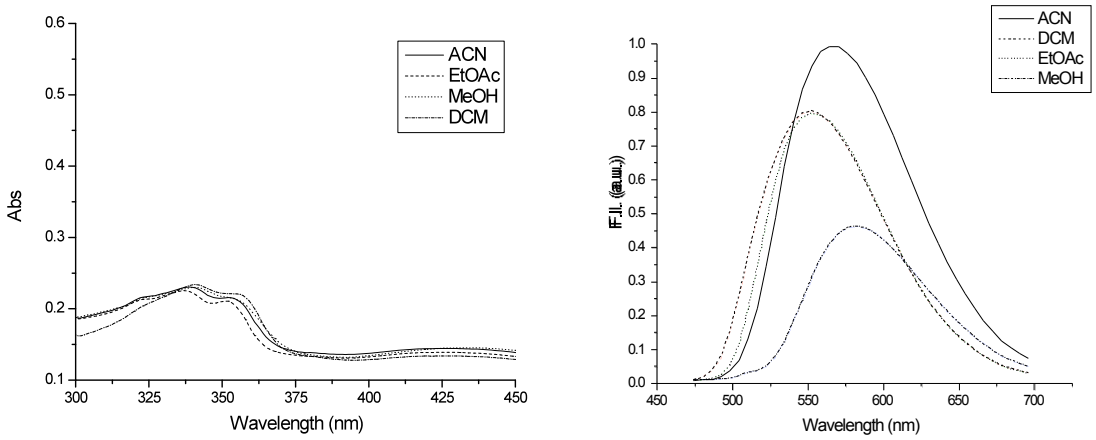
 (**5**) 4-Sulfo-*N*-(4-amino phenyl)-1,8-NI	λmax (Abs)	λex (nm)	λem (nm)	F.Intensity (a.u.)	Quantum yield
Dichloromethane M = 1.0 x 10^{-5}	350 (0.230)	340	426	9.18 x10^{5}	1.3 x10^{-3}
Acetonitrile M = 1.0 x 10^{-5}	338 (0.287)	340	430	1.7 x10^{6}	1.9 x10^{-3}
Ethyl Acetate M = 1.0 x 10^{-5}	351 (0.243)	340	426	1.6 x10^{6}	2.1 x10^{-3}
Methanol M = 1.0 x 10^{-5}	336 (0.297)	340	434	3.1 x10^{6}	3.3 x10^{-3}



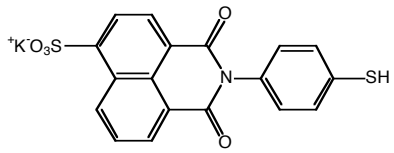
Supplementary Figure 2. Absorbance and fluorescence spectra of (**5**) 4-Sulfo-*N*-(4'-aminophenyl)-1,8-NI.

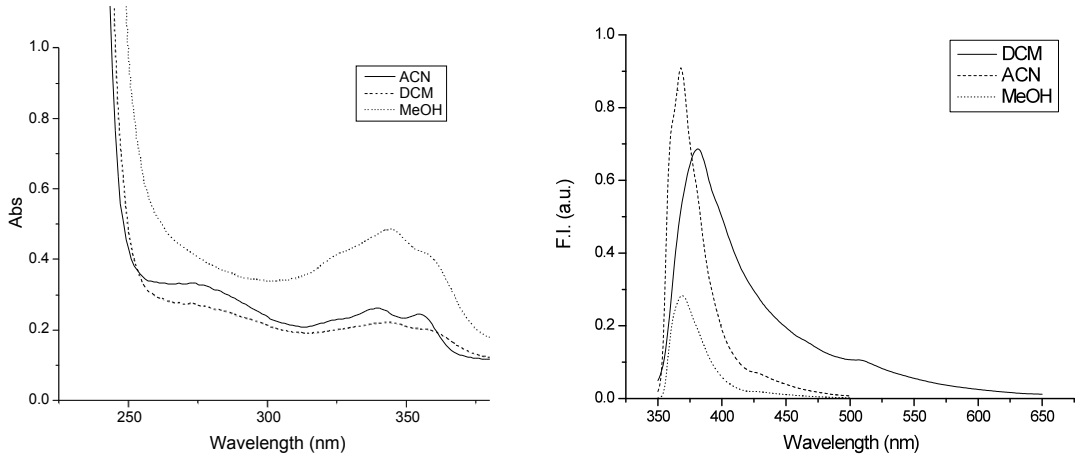
 (**6**)-4-Chloro-*N*-(4-amino phenyl)-1,8-NI	λmax (Abs)	λex (nm)	λem (nm)	F.Intensity A.U.	Quantum yield
Dichloromethane M = 1.0 x 10^{-5}	340 (0.346)	340	437 569	2.75 x10^{5} 4.11x10^{6}	2.5 x10^{-4} 3.8 x10^{-3}
Acetonitrile M = 1.0 x 10^{-5}	342 (0.240)	342	437 575	2.07 x10^{5} 2.46 x10^{5}	2.8 x10^{-4} 3.3 x10^{-4}
Ethyl Acetate M = 1.0 x 10^{-5}	342 (0.217)	342	426 564	1.24 x10^{5} 1.99 x10^{5}	1.8 x10^{-4} 2.9 x10^{-4}
Methanol M = 1.0 x 10^{-5}	342 (0.227)	342	434	2.34 x10^{5} 9.55 x10^{4}	3.3 x10^{-4} 1.3 x10^{-4}

 (**7**) 4-Cyano-*N*-(4'-thiophenyl)-1,8- NI	Absorbance	λex (nm)	λem (nm)	F.Intensity (a.u.)	Quantum yield
DCM M = 1.0 x 10^{-5}	342(0.235) 410(0.140)	410	553	17.3 x10^{6}	1.7 x10^{-2}
ACN M = 1.0 x 10^{-5}	340(0.274) 410(0.135)	410	567	9.2x10^{6}	2.2 x10^{-2}
EtOAc M = 1.0 x 10^{-5}	338(0.226) 410(0.136)	410	553	7.4 x10^{6}	1.7 x10^{-2}
MeOH M = 1.0 x 10^{-5}	341(0.230) 410(0.138)	410	582	4.3 x10^{6}	1.0 x10^{-2}

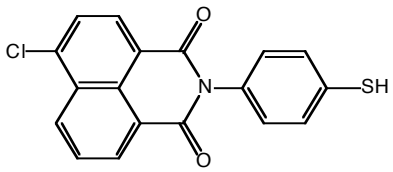


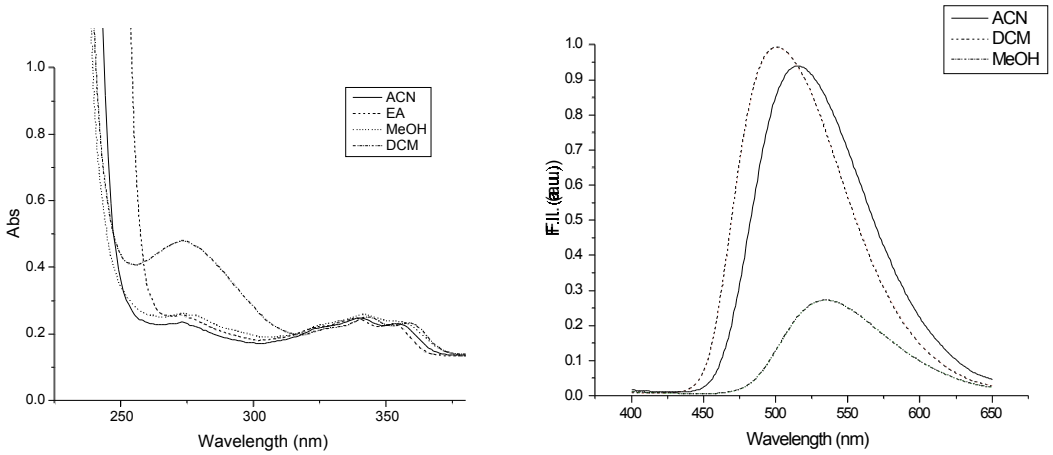
Supplementary Figure 3. Absorbance and fluorescence spectra of (**7**) 4-Cyano-*N*-(4'-thiophenyl)-1,8-NI.

 (**8**) 4-Sulfo-*N*-4-thiophenyl-1,8-NI	λmax (Abs)	λex (nm)	λem (nm)	F. Intensity A.U.	Quantum yield
Dichloromethane M = 1.0 x 10^{-5}	344 (0.221)	340	388	1.1 x10^{6}	1.6 x10^{-3}
Acetonitrile M = 1.0 x 10^{-5}	340 (0.262)	340	386	1.8 x10^{6}	2.2 x10^{-3}
MeOH M = 1.0 x 10^{-5}	342 (0.245)	340	386	1.8 x10^{6}	2.2 x10^{-3}



Supplementary Figure 4. Absorbance and fluorescence spectra of (**8**) 4-Sulfo-*N*-(4'-thiophenyl)-1,8-NI.

 (**9**) 4-Chloro-*N*-(4'-thiophenyl)-1,8-NI	λmax (Abs)	λex (nm)	λem (nm)	F. Intensity A.U.	Quantum yield
Methanol M = 1.0 x 10^{-5}	343 (0.251)	343	538	2.07 x10^{6}	2.6 x10^{-3}
Acetonitrile M = 1.0 x 10^{-5}	342 (0.247)	343	515	7.01 x10^{6}	9.1 x10^{-3}
Dichloromethane M = 1.0 x 10^{-5}	343 (0.251)	343	500	7.54 x10^{6}	9.6 x10^{-3}



Supplementary Figure 5. Absorbance and fluorescence spectra of (**9**) 4-Chloro-*N*-(4'-thiophenyl)-1,8-NI.