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Balancing the Molecular Twist and Conformational Rigidity In Imidazo[1,2-a]pyridine to achieve Dual-State Emissive (DSE) Luminogens for Applications in OLED and Cell-imaging

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General aspects:

All target molecules were synthesised via name reactions like Grindstone Chemistry, Heck reaction, Buchwald-Hartwig Cross Coupling Reaction, Knoevenagel Condensation Reaction, 1,4-Michael Addition Reaction and commercially available chemicals. These chemicals were parched form commercial sources like Sigma-Aldrich, Spectrochem, S. D. Fine chemicals, BLDpharma, Avra, Oxford and used without further purification. Reaction completion was monitor via Thin Layer Chromatography (TLC) using Silica gel-coated aluminium sheets (ACME, 254F) and EtOAc, petroleum ether as eluents. Product analysis carried out using Fourier transform infrared (FTIR) (ATR-IR) spectra which is obtained with Alpha-II/Bruker-instrument. ^{1}H Nuclear Magnetic Resonance (^{1}H NMR) spectroscopy was carried out on Bruker 400 and 500 MHz spectrometer whereas ^{13}C NMR was carried out on 100 MHz spectrometer using $CDCl_3$ as a solvent. Chemical shifts were reported in parts per million (ppm) downfield from TMS, and the spin multiplicities are described as s (singlet), d (doublet), t (triplet), and multiplet (m). Coupling constant (J) values are reported in hertz (Hz). Thermogravimetric analysis (TGA) was conducted on a Perkin-Elmer Diamond TG/DTA instrument at a heating rate of 10 °C/min under a nitrogen atmosphere with a 150 mL/min flow rate. UV-Visible absorption spectra were obtained on a FP-8200/Jasco spectrophotometer and emission spectra were obtained on FP-8200/Jasco spectrofluorometer. Redox potential is determined using PS-091 Cyclic voltammeter (Admiral Instruments) using 0.1M solution of tetrabutylammonium hexafluorophosphate ($^t Bu_4NPF_6$) in tetrahydrofuran (0.1 M) as an electrolyte, platinum gauze and Ag/AgCl as a counter and reference electrodes respectively with a scan rate of 25 mV/s. Solid state emission performed on FP-8200/Jasco spectrofluorometer. DFT studies of luminogens obtained via B3LYP functional with basis set 6-311++ G (d, p) using the Gaussian16 programme. Time-resolved fluorescence measurements were measured using a time-correlated single photon counting (TCSPC) unit (Horiba Deltaflex). The laser used for all the samples was of 510 nm. All the measurements were undergone at room temperature. The decay fitting was done by keeping the χ^2 value close to 1. Phosphorescence lifetime, gated emission and time-resolved excitation and emission were measured on FLS1000 spectrometer, Edinburgh Instruments equipped with a micro flash-lamp (µF2) set-up. Fluorescence lifetimes were performed on the same instrument. A 405 nm laser diode with a pulse repetition rate of 20 MHz were used as the light sources. Quantum yields were measured using an integrating sphere in the same instrument. Dynamic Light Scattering (DLS) studies were performed to measure partial size distribution in solutions by analysing the fluctuations in scattered light caused by Brownian motion. Studies perform on Malvern Zetasizer Nano-ZS90 instrument using sample evolving aggregates in THF at high water fraction. Dulbecco's modified eagle's media (DMEM), trypsin-EDTA solution (0.25% trypsin and 0.02% EDTA in DPBS), fetal bovine serum (FBS), dulbecco's phosphate-buffer saline (DPBS), and antibiotic antimycotic solution (10000 units of penicillin, 10.0 mg of streptomycin, and 25 µg of amphotericin B per mL in 0.9% normal saline), dimethyl sulfoxide (DMSO) (≥99.5%), trypan blue, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT), and tetrahydrofuran (THF), and 37% formaldehyde solution were purchased from HiMedia Laboratories Pvt. Ltd. Propidium iodide (PI) and 4´, 6-diamidino-2-phenylindole (DAPI) were procured from Merck Ltd., India. 2´, 7´-dichlorofluorescin diacetate (DCFDA), 30% hydrogen peroxide were supplied by Sigma Aldrich. Mouse fibroblast (L929) and human cervical cancer cell lines (SiHa) were procured from NCCS, Pune, India. The cells were cultured with complete

DMEM (DMEM supplemented with 10% v/v FBS and 1% v/v antibiotic antimycotic solution), and the incubation conditions were 37°C and 5% CO_2.

Synthetic Procedures and Characterization Data of 3a, 3b, 7 and SK-1 to SK-6.

Synthesis of phenyl(2-phenylimidazo[1,2-a]pyridin-3-yl)methanone (SK-1)[1]*:* A clean oven dried 25 ml RB flask, was charged with a magnetic stir bar and 1,3-diphenyl-2-propen-1-one (1.5 g, 7.20 mmol), 2-aminopyridine **1** (0.806 g, 8.57 mmol), $CuCl_2.2H_2O$ (0.096 g, 0.72 mmol) and toluene (10 ml) were added sequentially. The resulting solution was then refluxed at 120 ℃ for 12 hours under ambient air. On completion, the reaction mass was evaporated to dryness. The crude residue was purified by column chromatography (EtOAc/ Hexane) to obtain pure phenyl(2-phenylimidazo[1,2-a]pyridin-3- yl)methanone **(SK-1)** 1.28 g in 59% yield; Melting point: 132°C; IR: 3063, 1597, 1385, 1326, 886 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.55 (d, *J* = 6.9 Hz, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.53 (dd, *J* = 13.6, 7.6 Hz, 3H), 7.32 (d, *J* = 7.2 Hz, 2H), 7.27 – 7.23 (m, 1H), 7.17 – 7.04 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$): 186.3, 153.9, 146.4, 137.6, 132.9, 130.7, 129.1, 128.5, 128.2, 127.2, 126.7, 119.0, 116.4, 113.6.

Synthesis of 2-phenylimidazo[1,2-a]pyridine (3a)[2] : A mixture of 2-aminopyridine **1** (2.36 g, 25.1 mmol) and phenacyl bromide **2** (2 g, 10.0 mmol) was gently grounded in a mortar pestle at room temperature. The reaction mixture turned into a light-yellow solid mass within 3-5 minutes. After completion of the reaction as indicated by TLC, the reaction mixture was quenched with water followed by filtration and thoroughly washed with water to afford 2-phenylimidazo[1,2-a]pyridine **4** (1.76 g) in 90 % yield. The product was confirmed with the reported literature.

Synthesis of 2-(4-bromophenyl)imidazo[1,2-a]pyridine (3b)[2]: A mixture of 2-aminopyridine **1** (3.6 g, 38.3 mmol) and 4-bromophenacyl bromide **3** (3 g, 10.7 mmol) was gently ground in a mortar at room temperature. The reaction mixture turned into a light-yellow solid mass within 3-5 minutes. After completion of the reaction as indicated by TLC, the reaction mixture was quenched with water followed by filtration and washed thoroughly with water to afford the pure 2-(4-bromophenyl)imidazo[1,2-a]pyridine **5** (2.94 g) in 98 % yield. The product was confirmed by comparing it with the reported literature.

Synthesis of phenyl (4-(2-phenyl imidazo (1,2-a) pyridine-3-yl)phenyl) methanone (SK-2): In a 25 ml pressure tube, charged with a magnetic stir bar, 10 ml of *N, N* –dimethylacetamide was added with nitrogen purging followed by the addition of **4** (1g, 5.14 mmol), 4-bromo benzophenone **9** (1.34 g, 5.14 mmol), pivalic acid (0.15 g, 1.54 mmol), PCy_3HBF_4 (0.189 g, 0.514 mmol), $Pd(OAc)_2$ (0.05 g, 0.257 mmol) and K_2CO_3 (1.4 g, 10.2 mmol). After the addition, the tube was purged with nitrogen, sealed, and heated at 120 ℃ for 24 hours. The reaction mixture was cooled to room temperature, poured into ice-cold water, and extracted with ethyl acetate. The organic phase was dried over Na_2SO_4. The evaporation of the organic solvent gave a crude product which was further purified, with column chromatography using *n*-hexane and ethyl acetate as eluent. After purification, 1.52 g of phenyl (4-(2-phenyl imidazo[1,2-a] pyridine-3-yl)phenyl)methanone **SK-2** was obtained in 78 % yield; Melting point: 166°C ; IR: 3053, 1648, 1252, 914, 694 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 6.9 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 2H), 7.90 – 7.84 (m, 2H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.68 – 7.58 (m, 5H), 7.53 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.23 (m, 5H), 6.81 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): 195.0, 144.3, 142.5, 136.3, 133.1, 132.8, 131.7, 130.1, 129.3, 129.0, 127.4, 126.8, 124.1, 122.0, 118.9, 116.8, 111.7; HRMS: Calcd. for $C_{26}H_{17}N_2O$ (M^++H): 375.1497; found 375.1538.

Synthesis of 2-(phenyl(4-(2-phenylimidazo[1,2-a]pyridin-3-yl)phenyl)methylene)malononitrile (SK-3): In two neck round bottom flask fitted with a magnetic stir bar, phenyl (4-(2-phenyl imidazo (1,2-a) pyridine-3-yl)phenyl) methanone **SK-2** (0.75 g, 2.0 mmol) and malononitrile (0.54 ml, 9.7 mmol) were added and dissolved in pyridine (10 ml). The reaction mixture was then refluxed at 120 °C for 3 hours. The reaction was continuously monitored via TLC. After completion of the reaction, as indicated by the disappearance of the starting material, the reaction was cooled, diluted with water, and extracted with ethyl acetate. The organic phase was dried over Na_2SO_4. Evaporation of the solvent gave the crude product which was then purified by silica gel column chromatography using *n*-hexane and ethyl acetate as eluent to obtain 0.47 g of phenyl (4-(2-phenylimidazo (1,2-a) pyridine-3-yl)phenyl)methylene) malononitrile **(SK-3)** in 55% yield. Melting point: 256°C; IR: 3045, 2230, 1660, 1629, 695 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.14 (d, *J* = 6.9 Hz, 1H), 7.72 (d, *J* = 9.1 Hz, 1H), 7.64 – 7.58 (m, 7H), 7.55 – 7.49 (m, 4H), 7.35 – 7.25 (m, 5H), 6.83 (td, *J* = 6.8, 1.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): 172.8, 144.5, 143.1, 134.7, 133.5, 132.6, 131.8, 130.5, 129.4, 128.0, 127.4, 127.0, 124.5, 122.0, 118.4, 116.9, 112.8, 112.0; HRMS: Calcd. for $C_{29}H_{18}N_4$ (M^++H): 423.1609; found, 423.1631.

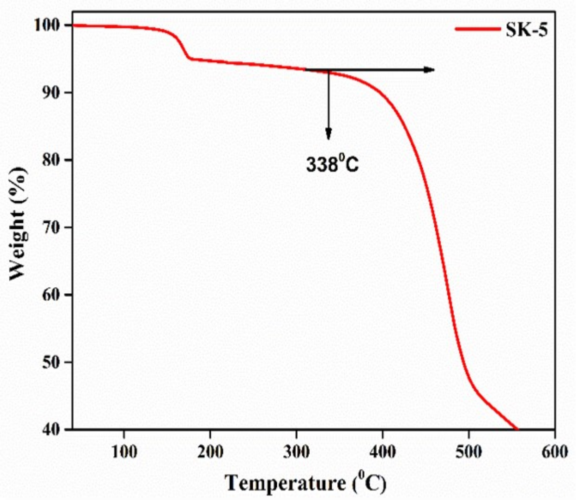
Synthesis of 4-(imidazo[1,2-a]pyridin-2-yl)-*N,N*-diphenylaniline (7)[3]: In a 2-necked oven-dried round bottom flask equipped with condenser and magnetic stir bar, 20 ml toluene was taken which was further charged with 2-(4-bromophenyl)imidazo[1,2-a]pyridine **5** (2 g, 7.32 mmol) and diphenylamine **6** (1.32 g, 7.32 mmol), under nitrogen atmosphere. The reaction mixture was stirred for 10 min and then $P(t\text{-}Bu)_3$ (0.61 ml, 2.63 mmol), $Pd(OAc)_2$ (0.16 g, 0.732 mmol), and K_2CO_3 (10.1 g, 73.2 mmol) were added sequentially followed by refluxing for 24 hours at 115 °C. After completion of the reaction, as observed from the TLC analysis, the solvent was evaporated under reduced pressure, and water was added to the reaction mixture and extracted in ethyl acetate. The organic layer was washed with saturated brine solution and dried over anhydrous sodium sulfate. The organic layer was evaporated under reduced pressure to get hold of the crude product which was further purified by silica gel column chromatography using petroleum ether and ethyl acetate as eluent to obtain 1.2 g of 4-(imidazo[1,2-a]pyridin-2-yl)-N,N-diphenylamine **(7)** in 78% yield. Product formation was confirmed by comparing with the reported literature.

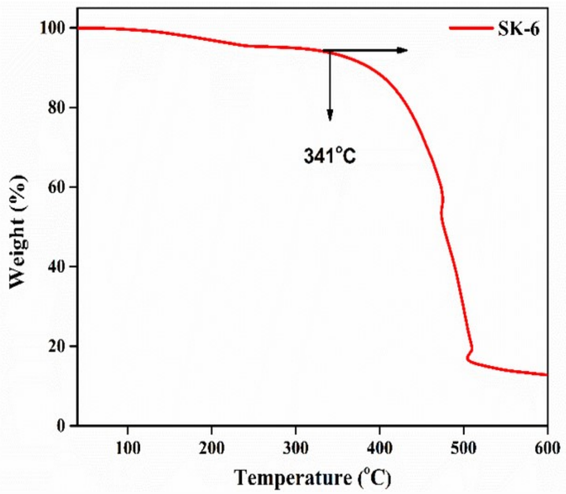
Synthesis of (4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methanone (SK-4): In a 15 ml pressure tube, charge with a magnetic stir bar, 6 ml of DMA was taken with nitrogen purging followed by sequential addition of 4-(imidazo[1,2-a]pyridin-2-yl)-*N,N*-diphenylaniline **7** (0.6 g, 3.09 mmol), 4-bromobenzophenone **9** (0.806 g, 3.09 mmol), pivalic acid (0.094 g, 0.92 mmol), PCy_3HBF_4 (0.113 g, 0.309 mmol), $Pd(OAc)_2$ (0.034 g, 0.154 mmol) and K_2CO_3 (0.85 g, 0.18 mmol). After addition, the tube was purged with nitrogen, sealed, and heated at 120 °C for 24 hours. After completion, the reaction mixture was dumped into ice-cold water and extracted with ethyl acetate, and the organic phase was dried over Na_2SO_4 and filtered. The evaporation of the solvent gave crude products which were further purified by silica gel column chromatography using *n*-hexane and ethyl acetate as eluent. After purification, 0.625 g of (4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methanone **(SK-4)** was obtained in 69% yield; Melting point: 200°C; IR: 2913, 1650, 1478, 1270, 691 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.05 (d, *J* = 6.9 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 2H), 7.87 (d, *J* = 7.3 Hz, 2H), 7.68 (d, *J* = 9.1 Hz, 1H), 7.66 – 7.59 (m, 3H), 7.56 – 7.49 (m, 4H), 7.24 (dd, J_1 = 14.1 Hz and J_2 = 6.5 Hz, 6H), 7.11 (d, *J* = 7.8 Hz, 4H), 7.01 (t, *J* = 8.2 Hz, 4H), 6.78 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): 196.0, 147.5, 145.2, 143.2, 137.3, 134.4, 132.6, 131.2, 130.4, 130.0, 129.4, 129.3, 129.0, 128.4, 127.5, 124.6, 123.0, 119.3, 117.6, 112.5; HRMS: Calcd. for $C_{38}H_{27}N_3O$ (M^++H), : 542.2232; found 542.2204.

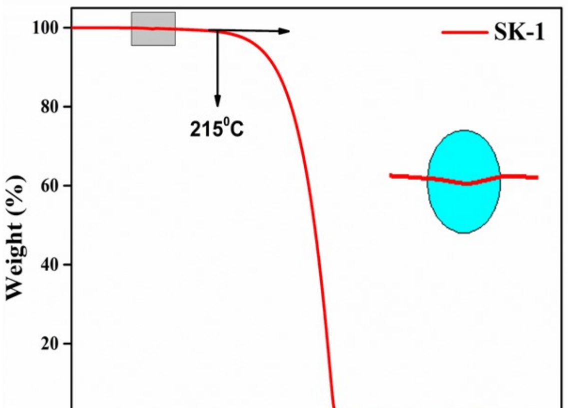
Synthesis of 2-((4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methylene)malononitrile (SK-5): In a two neck round bottom flask fitted with a magnetic stir bar, (4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methanone **SK-4** (0.35 g, 0.64 mmol) and malononitrile (0.09 ml, 1.61 mmol) were taken and dissolved in 4 ml of pyridine. After mixing, the reaction mixture was refluxed at 120 °C for 3 hours. The reaction was continuously monitored via TLC to check the completion. After completion of the reaction, the reaction mixture was poured into water and extracted with ethyl acetate. The organic phase was dried over Na_2SO_4 and filtered. The evaporation of the solvent gave a crude product which was further purified by silica gel column chromatography using *n*-hexane and ethyl acetate as eluent. After purification, 0.076 g of pure 2-((4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methylene)malononitrile **(SK-5)** (0.22 g) was obtained in 57% yield**;** Melting point: 220°C; IR: 2933, 2217, 1585, 1481, 1264, 753, 689 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): 8.09 (d, *J* = 6.9 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.64 – 7.57 (m, 5H), 7.57 – 7.44 (m, 6H), 7.25 (dd, J_1 = 10.6 and J_2 = 5.0 Hz, 6H), 7.11 (d, *J* = 7.7 Hz, 4H), 7.04 – 6.96 (m, 3H), 6.81 (dd, *J* = 13.3, 6.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): 172.7, 146.6, 146.4, 144.4, 142.8, 134.8, 134.5, 133.8, 131.7, 130.6, 129.5, 129.3, 128.2, 128.0, 126.2, 124.3, 123.7, 122.1, 121.8, 117.7, 116.6, 112.8, 111.8; HRMS: Calcd. for $C_{41}H_{27}N_5$ (M^++H) : 590.2344; found: 590.2331.

Synthesis of 3-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)-9H-fluoren-9-one (SK-6): In a 15 ml seal tube fitted with a magnetic stir bar, 5 ml of dimethyl acetamide was taken with nitrogen purging, followed by sequential addition of 4-(imidazo[1,2-]pyridin-2-yl)-*N, N*-diphenylaniline **7** (0.25 g, 3.09 mmol), 4-bromobenzophenone **9** (0.33 g, 1.28 mmol), pivalic acid (0.03 g, 0.38 mmol), PCy_3HBF_4 (0.047 g, 0.12 mmol), $Pd(OAc)_2$ (0.01 g, 1.28 mmol) and K_2CO_3 (0.35 g, 2.56 mmol). After addition, the tube was sealed and refluxed at 120 °C for 24 hours. After completion of the reaction as confirmed by TLC, the reaction mixture was poured into ice-cold water and extracted with ethyl acetate, and the organic layer was given brine washing and dried over Na_2SO_4. Evaporation of the solvent gave the crude product which on further purification with silica gel column chromatography using *n*-hexane and ethyl acetate as eluent gave 0.15 g of 3-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)-9H-fluoren-9-one **SK-6** in 42 % yield; Melting point: 243°C; IR: 2918, 1712, 1482, 1257, 696 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$): 8.06 (d, *J* = 6.9 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.70 (dd, *J* = 12.0, 8.3 Hz, 2H), 7.62 (s, 1H), 7.58 (t, *J* = 6.9 Hz, 2H), 7.51 (q, *J* = 7.1 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.35 (td, J_1 = 7.3 and J_2 = 1.6 Hz, 1H), 7.28 – 7.17 (m, 5H), 7.09 (d, *J* = 7.7 Hz, 4H), 7.00 (dd, *J* = 12.3, 5.3 Hz, 4H), 6.80 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): 193.0, 147.6, 147.4, 145.6, 145.3, 143.7, 143.4, 136.6, 134.8, 134.4, 133.9, 131.1, 129.6, 129.2, 129.0, 127.4, 125.3, 125.1, 124.6, 123.1, 122.3, 120.5, 119.4, 117.6, 112.7; HRMS: Calcd. for $C_{38}H_{25}N_3O$ (M^++H): 540.2075; found 540.2014.

Thermogravimetric Analysis of SK-1- SK-6


SK-5
338°C
Weight (%)
100
90
80
70
60
50
40
100
200
300
400
500
600
Temperature (°C)


SK-6
341°C
Weight (%)
100
80
60
40
20
0
100
200
300
400
500
600
Temperature (°C)


SK-1
215°C
Weight (%)
100
80
60
40
20

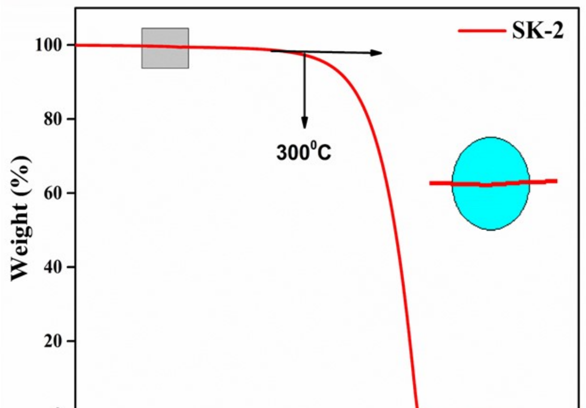

SK-2
300°C
Weight (%)
100
80
60
40
20

Figure. S1. TGA thermograms of **SK-1** to **SK-6.**

DSC Profiles of SK-1 to SK-6

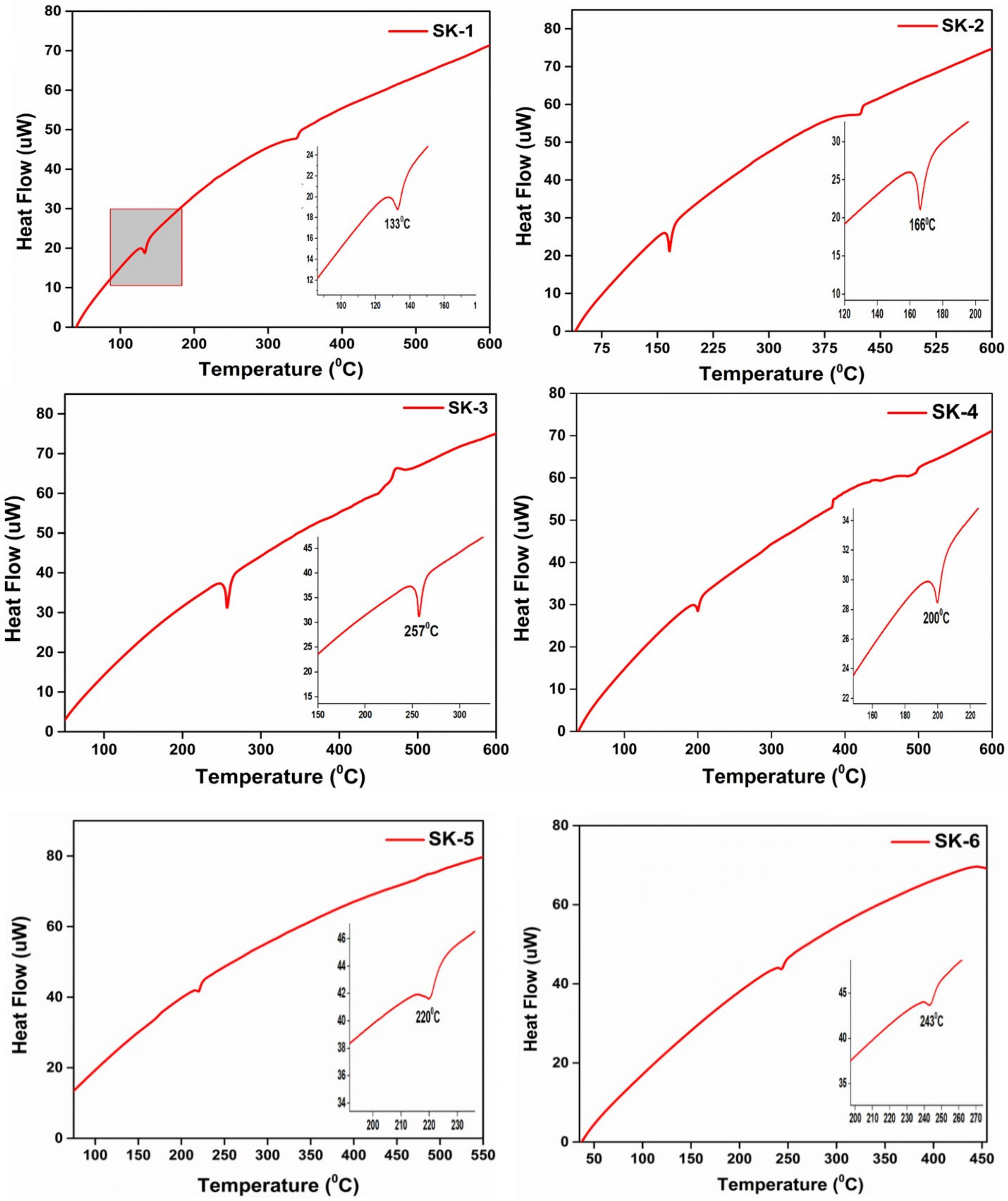


Figure. S2. DSC thermograms of SK-1 to SK-6.

Computational Details of SK-1 to SK-6

In the current study, we conducted a thorough geometry optimization of all the structures using the Gaussian 09 program. The calculations were performed at the DFT (Density Functional Theory) level, employing the B3LYP functional and the 6-311++G(d,p) basis set. Additionally, we investigated the impact of the solvent on the structures by carrying out single-point electronic structure calculations using an implicit CPCM model, specifically in the acetonitrile environment. The Cartesian coordinates for the optimized structure are provided.

SK-1

Total energy -955.25483527 a.u.

Charge: 0

Spin: Singlet

Dipole moment: 1.2575 Debye

Function/Basis set: B3LYP/6-311G

C	-4.47160000	2.10942700	0.11320800
C	-4.44829000	0.71881900	-0.18573600
C	-3.26289200	0.06908800	-0.43357300
N	-2.08595700	0.78750200	-0.37255200
C	-2.07619600	2.16933500	-0.09504000
C	-3.29514400	2.83005300	0.15575500
C	-0.73822300	0.38538300	-0.52295200
C	0.00670200	1.58769900	-0.40219100
N	-0.81566600	2.65124900	-0.12351000
C	1.43860900	1.84786900	-0.61857500
C	2.05518400	2.89409000	0.09553900
C	3.40256100	3.19606600	-0.11040100

C	4.15315200	2.46945800	-1.04347700
C	3.54311100	1.44393100	-1.77516600
C	2.19620400	1.13670200	-1.56781000
C	-0.41126200	-1.02027900	-0.72141400
O	-1.26273000	-1.80387500	-1.23599500
C	0.88990500	-1.58667700	-0.26139000
C	1.37651000	-2.73645300	-0.91094700
C	2.55313300	-3.34820300	-0.47688800
C	3.24468800	-2.83305200	0.62814900
C	2.75258100	-1.70570400	1.29636300
C	1.58299000	-1.08242800	0.85336900
H	-5.41949400	2.60156500	0.29860500
H	-5.37132600	0.15498200	-0.23723400
H	-3.16733300	-0.97135200	-0.70220900
H	-3.26491100	3.88986900	0.37183000
H	1.46008900	3.46317500	0.80023500
H	3.86593500	4.00007100	0.45275100
H	5.19999500	2.70644700	-1.20551000
H	4.11252000	0.88827500	-2.51330100
H	1.72868800	0.35503100	-2.15524500
H	0.81454200	-3.13562800	-1.74780300
H	2.92831700	-4.22658300	-0.99215700
H	4.15718800	-3.31166700	0.96969400
H	3.27726300	-1.31331100	2.16129800
H	1.20175700	-0.21477400	1.37867900

SK-2

Total energy -1186.30112282 a.u.

Charge: 0

Spin: Singlet

Dipole moment: 4.1172 Debye

Function/Basis set: B3LYP/6-311G

C	-3.92018100	-5.74520700	1.11623600
C	-4.32268200	-4.45876300	0.64711600
C	-3.40544400	-3.45318500	0.48365000
N	-2.07864800	-3.69378900	0.78725100
C	-1.63891600	-4.97088600	1.22613200
C	-2.59499100	-5.99740500	1.39624800
C	-0.93960300	-2.88029800	0.68518300
C	0.13233600	-3.70031500	1.08037600
N	-0.31082100	-4.97153200	1.40272800
C	1.56220900	-3.38221900	1.21563500
C	2.49683900	-4.43619300	1.16290000
C	3.86289100	-4.18416200	1.29941500
C	4.32383900	-2.87665600	1.49875300
C	3.40337600	-1.82471700	1.57023200
C	2.03478900	-2.07334700	1.43367800
C	-1.00543900	-1.49974600	0.18603300
C	-1.89030900	-0.55642500	0.74912500

C	-1.95142500	0.75139800	0.26335800
C	-1.12977900	1.15756800	-0.80380100
C	-0.25839200	0.21235800	-1.38035800
C	-0.19032300	-1.08828200	-0.89204800
C	-1.19756100	2.51727500	-1.41626100
O	-0.89459100	2.66190400	-2.62490900
C	-1.62223700	3.70542800	-0.61755300
C	-2.19413600	4.79237500	-1.30680100
C	-2.56869900	5.94805500	-0.62147400
C	-2.35555200	6.04436900	0.76083200
C	-1.76354300	4.98077300	1.45137800
C	-1.40186500	3.81487500	0.76870300
H	-4.66369500	-6.52351200	1.24302200
H	-5.36137500	-4.26441200	0.40961600
H	-3.65282700	-2.46675700	0.11912100
H	-2.24527600	-6.96216700	1.74034300
H	2.12836300	-5.44526900	1.02151100
H	4.56855100	-5.00777400	1.25145500
H	5.38633000	-2.68097500	1.60439600
H	3.74919300	-0.80999100	1.74162000
H	1.33375200	-1.25135100	1.51589600
H	-2.51817800	-0.84397300	1.58659500
H	-2.65186900	1.45057100	0.70550100
H	0.34924700	0.51891500	-2.22413200
H	0.48778900	-1.80343000	-1.34387900

H	-2.33082500	4.70861000	-2.37904400
H	-3.01990400	6.77470600	-1.16060800
H	-2.64186400	6.94566400	1.29364200
H	-1.57786000	5.06036300	2.51765000
H	-0.92229300	3.00503100	1.30674000

SK-3

Total energy -1334.80211771 a.u.

Charge: 0

Spin: Singlet

Dipole moment: 6.5090 Debye

Function/Basis set: B3LYP/6-311G

C	-4.17171900	4.02687900	0.92339400
C	-4.07183100	2.60448800	0.86725800
C	-2.91309800	1.99820200	0.45593500
N	-1.83573900	2.78064500	0.08529100
C	-1.89138600	4.19804600	0.15793400
C	-3.09297400	4.81118500	0.57773700
C	-0.53927800	2.44299400	-0.33393600
C	0.12033700	3.67289900	-0.51099800
N	-0.71521000	4.73086200	-0.20177400
C	1.48422200	3.94646000	-0.98936600
C	2.10469900	5.15472200	-0.61308200
C	3.39199500	5.46194100	-1.05713800
C	4.08187600	4.57378800	-1.89204700

C	3.46769100	3.37967500	-2.28711400
C	2.17933600	3.06826100	-1.84365400
C	-0.08169700	1.05253400	-0.44198800
C	-0.80756900	0.08710400	-1.17095800
C	-0.36689200	-1.23362600	-1.25554100
C	0.82167800	-1.64067000	-0.61766500
C	1.54271000	-0.67789000	0.12272000
C	1.10399300	0.63991100	0.20441700
C	1.31730200	-3.03759200	-0.68850200
C	1.29984200	-3.73574300	-1.87272000
C	1.83200300	-3.64575900	0.56643700
C	3.04065900	-4.37021300	0.59729700
C	3.51045400	-4.91512800	1.79446500
C	2.77862700	-4.75607600	2.97724600
C	1.57792600	-4.03597100	2.96014600
C	1.11335400	-3.47574500	1.76852900
C	0.96440600	-3.15164600	-3.13610400
N	0.71877200	-2.71595700	-4.19913100
N	1.61948000	-5.08579500	-1.95029000
C	1.86192200	-6.24690800	-2.06848900
H	-5.09996800	4.48435000	1.24525200
H	-4.91405600	1.98622100	1.15268100
H	-2.78146900	0.92717400	0.40560700
H	-3.12150200	5.89238100	0.61770100
H	1.55604700	5.84166300	0.02045000

H	3.85637000	6.39538600	-0.75457000
H	5.08214900	4.81383900	-2.23864000
H	3.98563100	2.69479000	-2.95125000
H	1.70640500	2.15378500	-2.18192500
H	-1.71114400	0.37795200	-1.69647400
H	-0.95511600	-1.95189200	-1.81453200
H	2.45390400	-0.97091000	0.63206500
H	1.67503900	1.36449600	0.77341600
H	3.61929800	-4.49288900	-0.31058500
H	4.44725800	-5.46216400	1.80292100
H	3.14281800	-5.18579600	3.90467300
H	1.00598400	-3.90863900	3.87335500
H	0.18607000	-2.91331900	1.76045100

SK-4

Total energy -1703.73436296 a.u.

Charge: 0

Spin: Singlet

Dipole moment: 4.9078 Debye

Function/Basis set: B3LYP/6-311G

C	-6.37788200	4.49732500	0.02173400
C	-6.42616900	3.07262700	-0.03944200
C	-5.27215900	2.33303200	-0.07976900
N	-4.05271500	2.98237800	-0.06929300
C	-3.96788500	4.39729600	0.02066100

C	-5.16396300	5.14870000	0.05642900
C	-2.73756900	2.49127100	-0.06599100
C	-1.91917800	3.63421100	0.00773100
N	-2.68678700	4.78580600	0.06441300
C	-0.45574800	3.75059800	-0.00847900
C	0.13983400	4.92763100	0.49038400
C	1.52033300	5.10146300	0.47614000
C	2.36425500	4.09700100	-0.03791100
C	1.77713400	2.92386600	-0.54903300
C	0.39307100	2.76091300	-0.54188800
N	3.77907800	4.26785200	-0.04972500
C	4.54841000	3.80104500	-1.16220200
C	4.43833900	4.90424900	1.04775900
C	5.47862200	5.82362700	0.81673700
C	6.13012800	6.43421100	1.89120800
C	5.74753100	6.15307200	3.20854600
C	4.70748100	5.24447700	3.44058900
C	4.06136400	4.61637400	2.37303900
C	5.75727000	3.11219900	-0.95236700
C	6.51158100	2.66778700	-2.04122800
C	6.06755300	2.88735800	-3.35104100
C	4.86075800	3.56587700	-3.56182300
C	4.10803300	4.02812700	-2.47931100
C	-2.44114200	1.05279800	-0.07043900
C	-2.99171000	0.19118400	-1.04285900

C	-2.72770600	-1.17975500	-1.02194300
C	-1.89136600	-1.73294900	-0.03491300
C	-1.31371900	-0.87014900	0.91794600
C	-1.59428000	0.49187100	0.91218800
C	-1.51043700	-3.17506400	0.00253100
O	-0.41730900	-3.50811900	0.52034800
C	-2.40318200	-4.22815900	-0.56717000
C	-3.80561900	-4.10956700	-0.59951600
C	-4.59244600	-5.15861100	-1.08606600
C	-3.98878500	-6.33175300	-1.55267600
C	-2.59351800	-6.46251200	-1.51445200
C	-1.80820500	-5.42369700	-1.01477300
H	-7.30253200	5.06218400	0.04737200
H	-7.37927800	2.55822800	-0.05059000
H	-5.25067600	1.25350800	-0.11428700
H	-5.08239100	6.22632100	0.11605100
H	-0.50564800	5.71092500	0.86945000
H	1.95321300	6.01866000	0.85860000
H	2.40853800	2.14309200	-0.95688500
H	-0.02559200	1.85437500	-0.96164900
H	5.76883300	6.05446600	-0.20193000
H	6.93032100	7.14155500	1.69634000
H	6.25141700	6.63385800	4.04050200
H	4.40539300	5.01170700	4.45704100
H	3.26669200	3.90266800	2.55819600

H	6.09677400	2.92879300	0.06079900
H	7.44171700	2.13674300	-1.86410400
H	6.65254900	2.53499800	-4.19419500
H	4.50882500	3.74868800	-4.57240900
H	3.18100700	4.56517700	-2.64554000
H	-3.60236100	0.60433100	-1.83952200
H	-3.14146000	-1.81230900	-1.79892100
H	-0.64943000	-1.29574800	1.66142900
H	-1.16076500	1.13909500	1.66617800
H	-4.28219900	-3.21369000	-0.21800800
H	-5.67343600	-5.06244500	-1.09480400
H	-4.60059500	-7.14213200	-1.93629800
H	-2.12331500	-7.37424600	-1.86833600
H	-0.72949300	-5.51569700	-0.95744900

SK-5

Total energy -1852.27002302 a.u.

Charge: 0

Spin: Singlet

Dipole moment: 6.5498 Debye

Function/Basis set: B3LYP/6-311G

C	-6.41493500	3.68411000	0.48335100
C	-6.41831400	2.25853300	0.43279600
C	-5.24739600	1.55896400	0.29103200
N	-4.05501500	2.24951900	0.18738100

C	-4.01306100	3.66675500	0.26663500
C	-5.22607300	4.37688900	0.40717000
C	-2.72659100	1.80671900	0.07521900
C	-1.94718600	2.98020700	0.07252700
N	-2.74742700	4.10207900	0.19546600
C	-0.49686700	3.14700600	-0.08007600
C	0.10954100	4.32507800	0.40249600
C	1.47566800	4.54630300	0.25863900
C	2.29450200	3.59052900	-0.37602000
C	1.69393300	2.41721400	-0.87288600
C	0.32330500	2.20727100	-0.73490800
N	3.69344300	3.81057800	-0.52284900
C	4.36840500	3.38451200	-1.71167000
C	4.43486500	4.46782500	0.50885200
C	5.39809000	5.44024800	0.18214600
C	6.13087100	6.07157500	1.19028200
C	5.90606400	5.75784600	2.53634200
C	4.94303500	4.79550700	2.86421200
C	4.21739400	4.14692800	1.86185600
C	5.61614000	2.74016100	-1.62729200
C	6.27916700	2.33665500	-2.78916500
C	5.70400700	2.55319600	-4.04741700
C	4.45868600	3.18806900	-4.13290300
C	3.79644700	3.61010200	-2.97731400
C	-2.36929300	0.38493200	0.05175300

C	-2.99927500	-0.52532300	-0.82433500
C	-2.65682900	-1.87652900	-0.82901800
C	-1.66942900	-2.37559000	0.04495600
C	-1.04745500	-1.46798300	0.93212200
C	-1.38406100	-0.11840900	0.93026300
C	-1.28678900	-3.80605200	0.06436300
C	-1.13843800	-4.53236400	-1.10286000
C	-1.06546600	-4.43499500	1.39127700
C	0.03623800	-5.28100800	1.63304400
C	0.22260500	-5.86093300	2.88991800
C	-0.68871600	-5.61292000	3.92296600
C	-1.78394900	-4.76960700	3.69754600
C	-1.96592400	-4.17639700	2.44732900
C	-0.94122000	-5.95128500	-1.11622500
N	-0.79948100	-7.11614600	-1.17793700
C	-1.16788400	-3.93361600	-2.40378700
N	-1.16553700	-3.48168000	-3.48852900
H	-7.35280000	4.21688300	0.58869800
H	-7.34973700	1.71114500	0.50920300
H	-5.19397800	0.48061300	0.26077000
H	-5.17654900	5.45696900	0.45546800
H	-0.51764500	5.07316200	0.87273700
H	1.91568700	5.46420900	0.63060400
H	2.30292100	1.67610000	-1.37709500
H	-0.10963500	1.30635700	-1.15315500

H	5.56515500	5.69556800	-0.85807900
H	6.86997700	6.82022200	0.92244700
H	6.47213200	6.25500200	3.31710000
H	4.76393700	4.53752900	3.90344000
H	3.48277600	3.39230200	2.11923000
H	6.05743600	2.55988500	-0.65349700
H	7.24118800	1.84010500	-2.70897300
H	6.21789400	2.23202500	-4.94735600
H	4.00525900	3.36778400	-5.10266000
H	2.83890700	4.11365200	-3.04803300
H	-3.74356500	-0.16718400	-1.52770300
H	-3.16741500	-2.54717100	-1.50974100
H	-0.29160900	-1.82923300	1.62031000
H	-0.88959300	0.56204400	1.61379600
H	0.75614300	-5.46866200	0.84504900
H	1.07978100	-6.50309200	3.06159900
H	-0.54445000	-6.06904600	4.89687600
H	-2.49407800	-4.57427900	4.49423100
H	-2.81473300	-3.52336200	2.27687900

SK-6

Total energy -1702.53386654 a.u.

Charge: 0

Spin: Singlet

Dipole moment: 2.2624 Debye

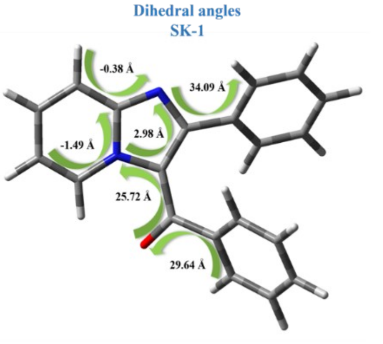
Function/Basis set: B3LYP/6-311G

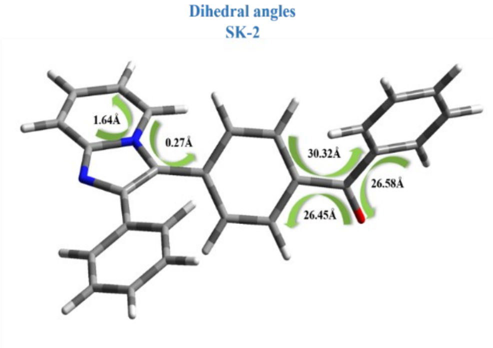
C	3.64679900	5.24784300	-5.92699300
C	4.53847400	4.14716100	-6.09799400
C	4.37604300	2.99390200	-5.37424100
N	3.33917900	2.90762900	-4.46474800
C	2.41538800	3.97224300	-4.29216900
C	2.59681500	5.15776000	-5.03919800
C	2.91710000	1.85913900	-3.63144200
C	1.76741600	2.34705200	-2.98172800
N	1.47461300	3.63407100	-3.40027500
C	0.92334400	1.71898200	-1.95772400
C	1.36767200	0.67741700	-1.11969000
C	0.53158100	0.12167400	-0.15291000
C	-0.77909900	0.60405200	0.02623700
C	-1.22209100	1.66281600	-0.79147600
C	-0.38646200	2.20464100	-1.76316200
N	-1.63361200	0.04085000	1.01780600
C	-3.02982700	-0.12473400	0.75735000
C	-1.09808500	-0.36560600	2.28121200
C	-1.48970100	-1.58700600	2.85965800
C	-0.97352200	-1.97665500	4.09816300
C	-0.04995200	-1.16657900	4.77020800
C	0.34678700	0.04592600	4.19268700
C	-0.17681900	0.45144800	2.96239700
C	-3.97942800	0.17575600	1.75179500

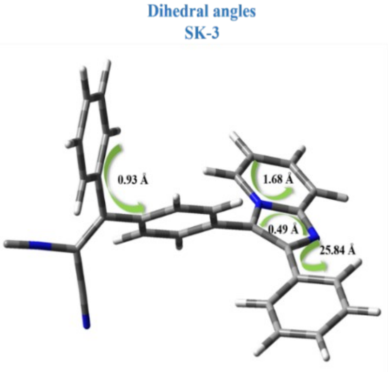
C	-5.34227300	-0.00071600	1.50027900
C	-5.78217500	-0.46208100	0.25351200
C	-4.83971900	-0.75416400	-0.74016500
C	-3.47389800	-0.59652700	-0.49219900
C	3.59789700	0.55770900	-3.60526500
C	2.85074200	-0.63168100	-3.81089900
C	3.50347600	-1.85591600	-3.79745400
C	4.90399500	-1.91786500	-3.59179900
C	5.65155700	-0.76620600	-3.38854300
C	4.99202100	0.47200400	-3.39213100
C	2.99791800	-3.24130300	-3.98209500
C	4.09473300	-4.13185000	-3.88563100
C	5.33974600	-3.34410400	-3.63724600
C	1.71709900	-3.73445800	-4.21175300
C	1.54734100	-5.12530600	-4.34462600
C	2.63622400	-6.00192900	-4.24856600
C	3.93006800	-5.50494700	-4.01553000
O	6.49568700	-3.78328000	-3.49942600
H	3.79797000	6.15197200	-6.50524000
H	5.35472600	4.21009300	-6.80706800
H	5.01427300	2.12784800	-5.47255500
H	1.88981600	5.96335700	-4.88887500
H	2.37783400	0.29773300	-1.21397500
H	0.89584700	-0.68415700	0.47358900
H	-2.22145400	2.06006700	-0.65617900

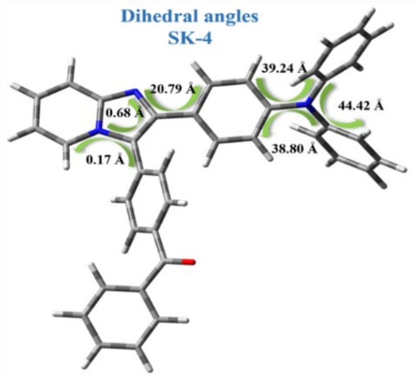
H	-0.72571500	3.03083300	-2.37652400
H	-2.19451900	-2.22254000	2.33559700
H	-1.28453200	-2.92206400	4.53174500
H	0.35419700	-1.47504900	5.72870300
H	1.05660100	0.68660400	4.70666700
H	0.12222200	1.39722900	2.52479100
H	-3.64401600	0.54616800	2.71382100
H	-6.06222000	0.23623900	2.27749300
H	-6.84175900	-0.59143900	0.05930100
H	-5.16655400	-1.11880200	-1.70912900
H	-2.74732000	-0.83694300	-1.26002700
H	1.78187000	-0.56017400	-3.97858300
H	6.72146600	-0.82941900	-3.21864500
H	5.55482200	1.37933200	-3.19897400
H	0.86150200	-3.07113700	-4.28702500
H	0.55415800	-5.52473200	-4.52407300
H	2.47761700	-7.06996900	-4.35423100
H	4.78441500	-6.16931200	-3.93713300

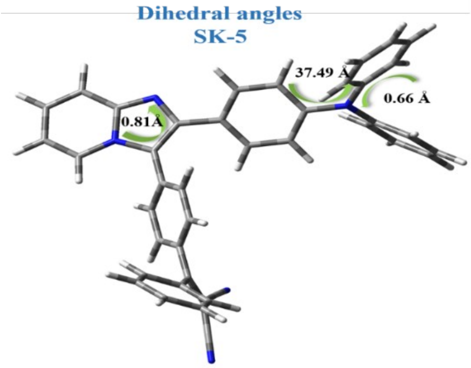
Energy Minimized Structures of SK-1 to SK-6

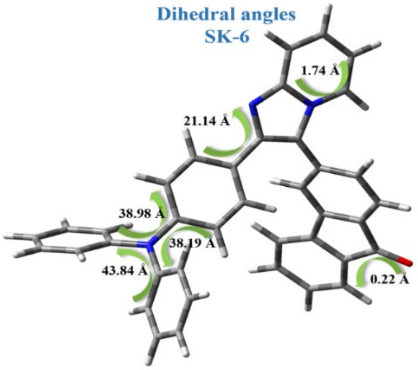






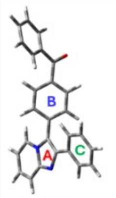




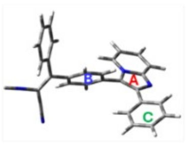


Energy Minimized Structure

SK-1



SK-2



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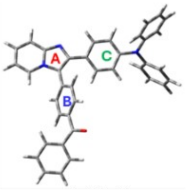
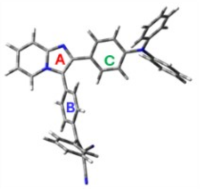
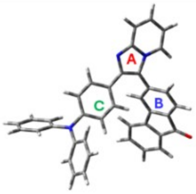


SK-4



SK-5



SK-6

Figure S3. Energy minimized structures of **SK-1 to SK-6** with their dihedral angles.

Table S1. Dihedral angles existing in **SK-1** to **SK-6.**

	SK-1	**SK-2**	**SK-3**	**SK-4**	**SK-5**	**SK-5**
Dihedral angle between ring A and ring C	34.09°	21.99 °	25.84 °	20.99 °	23.99 °	21.14 °
Dihedral angle between ring A and ring B	31.43 °	58.72 °	55.25 °	52.24 °	51.98 °	56.29 °

Electrochemical Studies of SK-1 to SK-6

Cyclic Voltammetry Analysis of **SK-1~6:** The electrochemical studies including redox potential and theoretical band gap calculations was carried out by cyclic voltammetry studies. The measurements were recorded in an electrolyte solution of 0.1 M tetrabutylammonium hexafluorophosphate ($^tBu_4NPF_6$) in THF using Ag/AgCl as reference electrode and platinum gauze as the counter electrode. Glassy carbon electrode was used as a working electrode and the analysis was carried out at a scan rate of 25 mV/s. The concentration of all luminogens (analyte) used as 1 mM. To perform the experiment, the three-electrode system was subjected to a solution containing both analyte and electrolyte in 1:1 proportion.

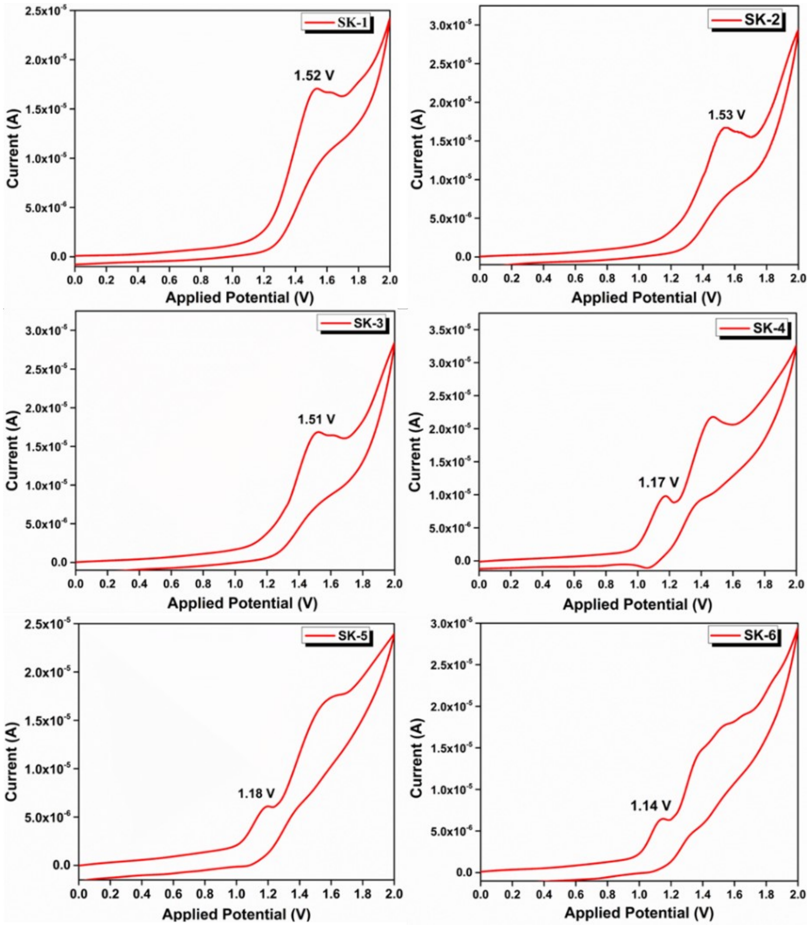


Figure. S4. Cyclic Voltamograms of **SK-1 to SK-6.**

Bandgap Calculations

HOMO and LUMO energies and HOMO-LUMO energy gap (EHL) of Luminogens **SK-1~6** calculated at DFT/B3LYP/6-311++ G (d, p) level.

$E_{\textbf{HOMO}}$ = − (4.8 + Eox onset) eV

$E_{\textbf{LUMO}}$ = E_{HOMO} + $E_{\text{band gap}}$ eV

Band gap = (E_{LUMO} – E_{HOMO}) eV or 1240/ $\lambda_{\text{max onset}}$

For **SK-1**

Onset absorption wavelength (λ_{max}) tetrahydrofuran: 342 nm

Onset CV oxidation: 1.52 V

E_{HOMO} = - (4.8 + E_{OX} onset) eV

= - (4.8 + 1.52) eV

= - 6.32 eV

$E_{\text{band gap}}$ = 1240/λ_{max}

= 1240/ 342

= 3.62 eV

$E_{LUMO} = E_{HOMO} + E_{band\ gap}$
$= -6.32 + 3.62$
$= -2.70$ eV

For **SK-2**

Onset absorption wavelength (λ_{max}) tetrahydrofuran: 338 nm

Onset CV oxidation: 1.53 V

$E_{HOMO} = - (4.8 + E_{OX}\ \text{onset})$ eV
$= - (4.8 + 1.53)$ eV
$= - 6.33$ eV

$E_{band\ gap} = 1240/\lambda_{max}$
$= 1240/338$
$= 3.66$ eV

$E_{LUMO} = E_{HOMO} + E_{band\ gap}$
$= -6.33 + 3.61$
$= -2.72$ eV

For **SK-3**

Onset absorption wavelength (λ_{max}) tetrahydrofuran: 405 nm

Onset CV oxidation: 1.51 V

$E_{HOMO} = - (4.8 + E_{OX}\ \text{onset})$ eV
$= - (4.8 + 1.51)$ eV
$= - 6.31$ eV

$E_{band\ gap} = 1240/\lambda_{max}$
$= 1240/405$
$= 3.07$ eV

$E_{LUMO} = E_{HOMO} + E_{band\ gap}$
$= -6.31 + 3.07$
$= -3.24$ eV

For **SK-4**

Onset absorption wavelength (λ_{max}) tetrahydrofuran: 346 nm

Onset CV oxidation: 1.17 V

$E_{HOMO} = - (4.8 + E_{OX}\ \text{onset})$ eV
$= - (4.8 + 1.17)$ eV
$= - 5.97$ eV

$E_{band\ gap} = 1240/\lambda_{max}$
$= 1240/346$
$= 3.58$ eV

$E_{LUMO} = E_{HOMO} + E_{band\ gap}$
$= -5.97 + 3.58$
$= -2.39$ eV

For **SK-5**

Onset absorption wavelength (λ_{max}) tetrahydrofuran: 450 nm

Onset CV oxidation: 1.18 V

E_{HOMO} = - (4.8 + E_{OX} onset) eV

= - (4.8 + 1.18) eV

= -5.98 eV

$E_{band\ gap}$ = 1240/λ_{max}

= 1240/450

= 2.75 eV

E_{LUMO} = E_{HOMO} + $E_{band\ gap}$

= -5.98 + 2.75

= -3.23 eV

For **SK-6**

Onset absorption wavelength (λ_{max}) tetrahydrofuran: 337nm

Onset CV oxidation: 1.14 V

E_{HOMO} = - (4.8 + E_{OX} onset) eV

= - (4.8 + 1.14) eV

= - 5.94 eV

$E_{band\ gap}$ = 1240/λ_{max}

= 1240/350

= 3.54 eV

E_{LUMO} = E_{HOMO} + $E_{band\ gap}$

= -5.94 + 3.54

= -2.40 eV

Photophysical Studies of SK-1 to SK-6

Preparation of stock solution luminogen SK-1 in THF solvent

Molecular weight = 298.35 g

Therefore, 298.35 g in 1000 mL of THF ≡ 1M

$$Concentration\ (M) = \frac{Mass\ (g)}{Formula\ weight\ (g) * Volume\ (L)}$$

Hence, to prepare 1mM stock solution 2.98 mg of **SK-1** was dissolved in 10 ml THF

Similarly stock solutions of **SK-2, SK-3, SK-4, SK-5, SK-6** were prepared.

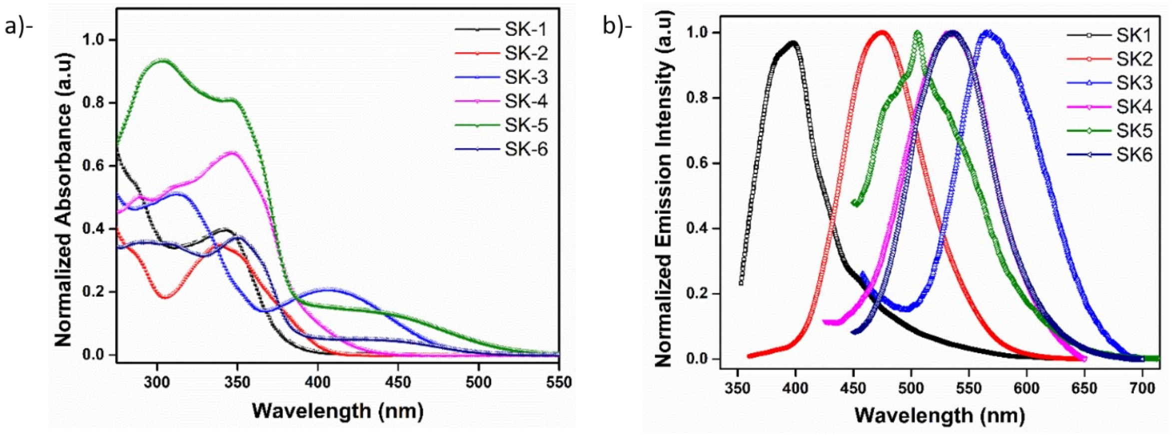


Figure. S5. a) Normalized absorption spectra of **SK-1 to SK-6** in THF solution; b) Normalized PL spectra of **SK-1 to SK-6** in THF solution (1 mM).

Solvatochromism studies of SK-1 to SK-6

To investigate the behavior of the luminogens in the presence of different solvents with graded polarity solvatochromism study was carried out where among the synthesized luminogens some are emissive in THF, so variation in this luminogens absorption or emission properties in different solvents was measured. It was observed that, **SK-1**, **SK-2** and **SK-3** shows change in emission intensity and wavelength shift according to change in polarity of different solvents. While **SK-4**, **SK-5**, **SK-6** shows emission only in hexane and show no interaction with other solvents with increase in solvent polarity.

Fluorescence Quantum Yield Calculation (Relative Method)

The fluorescence quantum yield of **SK-1** to **SK-6** was measured in different solvents in which they show Solvatochromism with respect to quinine sulphate which was taken as a standard (Φ = 0.54 in 0.1 M H_2SO_4).

$$\varphi_x = \varphi_{ST} * \frac{(Grad_x)}{(Grad_{ST})} * \frac{(\eta_x)^2}{(\eta_{ST})^2}$$

Here, ϕ_x = Quantum yield (**SK-1** to **SK-6**)
ϕ_{ST} = Quantum yield (quinine sulphate)

η_x = Refractive index of different solvents
η_{ST} = Refractive index of 0.1M H_2SO_4
In order to find out gradient for all this molecules, optical density (from UV) vs curve area (from emission) in solvent was plotted.

The absorption and emission wavelength of all luminogens were recorded in different solvents by keeping the absorption maxima to be < 0.1. Slowly concentration decreases by performing 50% dilution and readings were taken until it reaches to 0. The same followed for 0.1M quinin sulphate, which was diluted by 0.1M H_2SO_4. All values were recorded in UV-vis spectrophotometer and summarized in Table S1.

Table S2. Absorption, Emission and Quantum Yield data of **SK-1** to **SK-6** in solvents of various polarity.

Solvents	**Compounds**																	
	SK-1			**SK-2**			**SK-3**			**SK-4**			**SK-5**			**SK-6**		
	λ_{abs} (nm)	**λ_{em} (nm)**	**ϕ** (%)	**λ_{abs} (nm)**	**λ_{em} (nm)**	**ϕ** (%)	**λ_{abs} (nm)**	**λ_{em} (nm)**	**ϕ** (%)	**λ_{abs} (nm)**	**λ_{em} (nm)**	**ϕ** (%)	**λ_{abs} (nm)**	**λ_{em} (nm)**	**ϕ** (%)	**λ_{abs} (nm)**	**λ_{em} (nm)**	**ϕ** (%)
n-hexane	336	480	—	343	—	—	330	486	0.23	350	466	14.3	351	481	—	352	510	6.60
Toluene	---	—	—	342	454	—	318	545	0.44	350	501	17	354	—	—	354	558	1.97
$CHCl_3$	346	—	—	342	477	19.2	313	561	0.71	350	552	—	353	—	—	354	544	0.31
Acetone	343	—	—	343	491	12.9	318	—	—	344	496	—	346	—	—	—	—	—
ACN	343	—	—	340	504	7.80	318	—	—	343	—	—	344	—	—	345	—	—
DMSO	346	—	—	342	515	14	313	—	—	347	—	—	345	—	—	350	—	—
DMF	344	—	—	343	528	5.14	313	—	—	344	—	—	344	—	—	348	—	—

--- = not emissive enough to calculate quantum yield

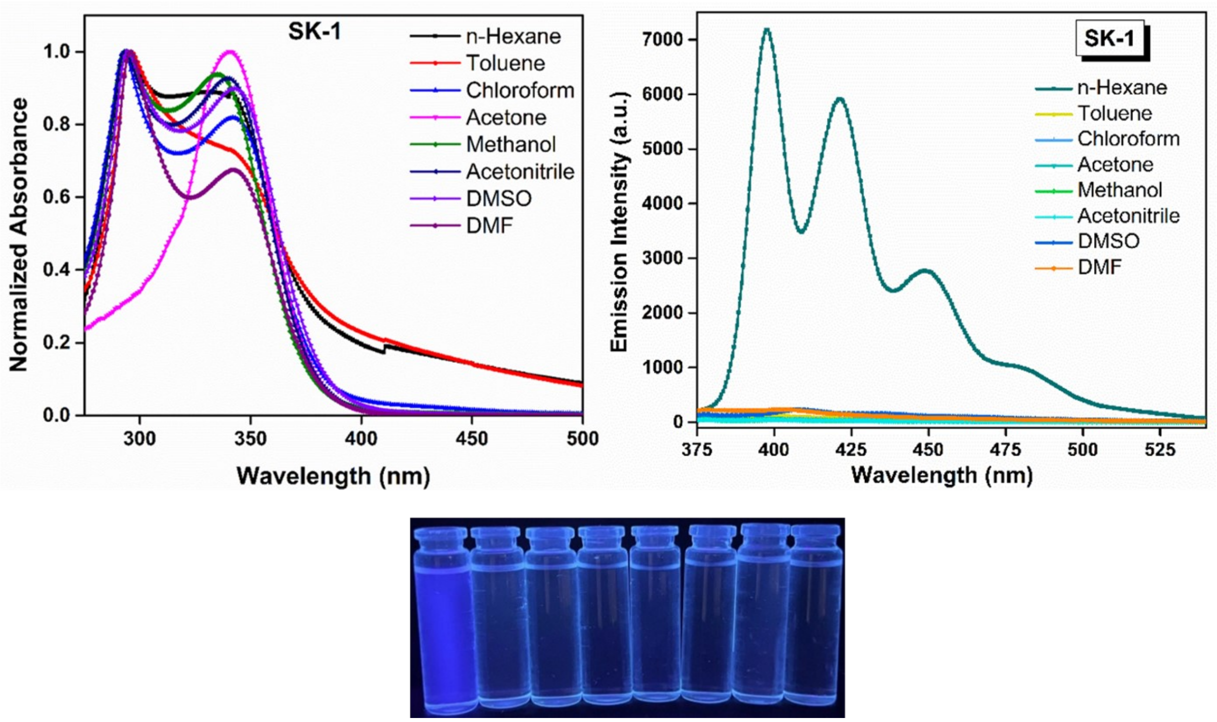


Figure S6. Absorption, and emission spectra of **SK-1** in solvents with graded polarity (From left: *n*-hexane, Toluene, Chloroform, Acetone, Methanol, Acetonitrile, DMSO, DMF).

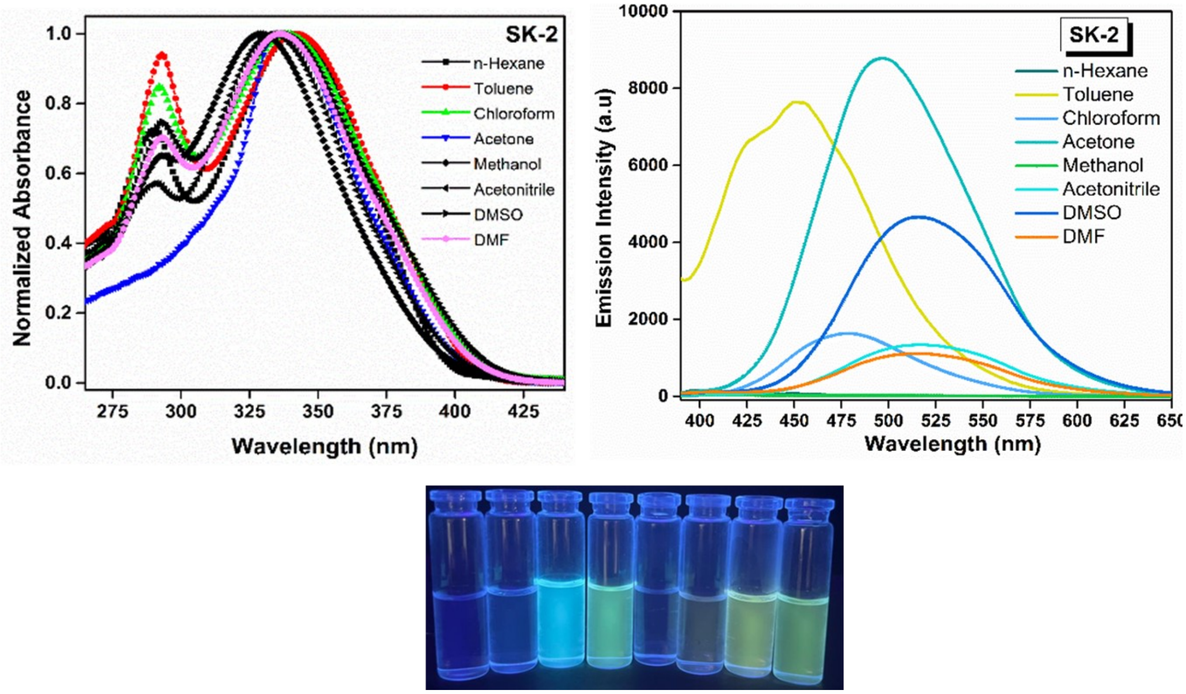


Figure. S7. Absorption, emission spectra of **SK-2** in solvents with graded polarity (From left: *n*-hexane, Toluene, Chloroform, Acetone, Methanol, Acetonitrile, DMSO, DMF).

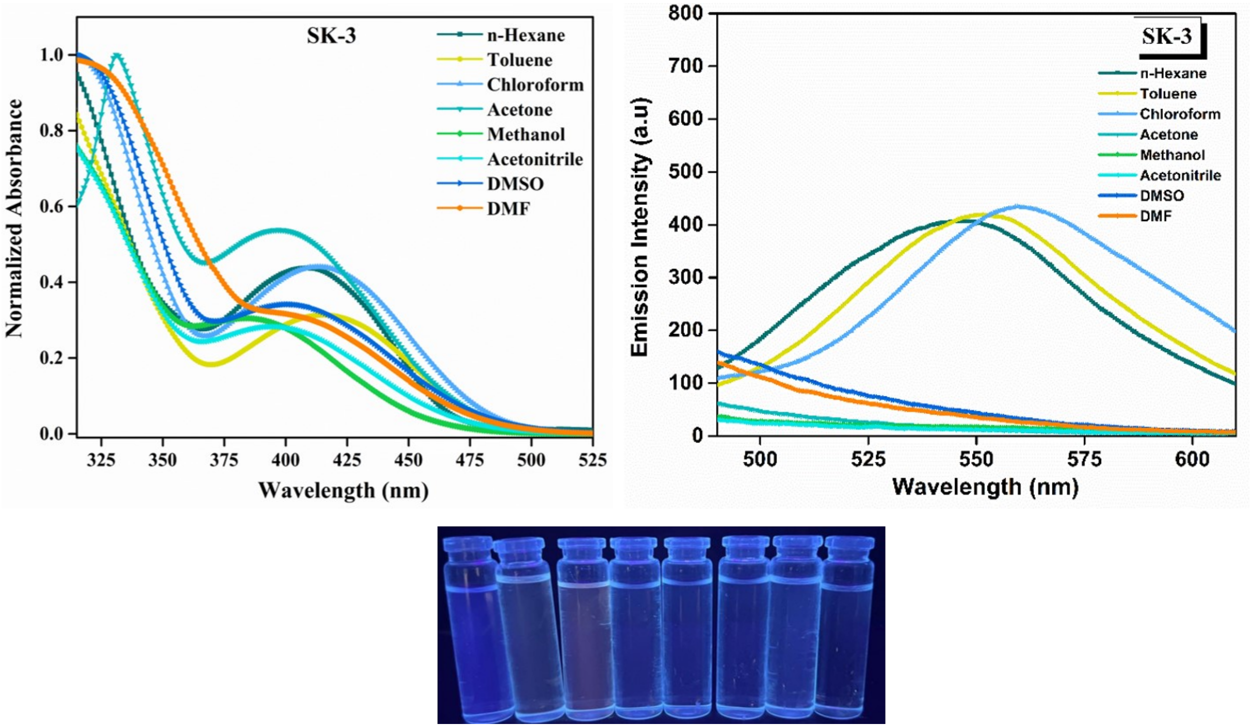


Figure. S8. Absorption, emission spectra of **SK-3** in solvents with graded polarity (From left: *n*-hexane, Toluene, Chloroform, Acetone, Methanol, Acetonitrile, DMSO, DMF).

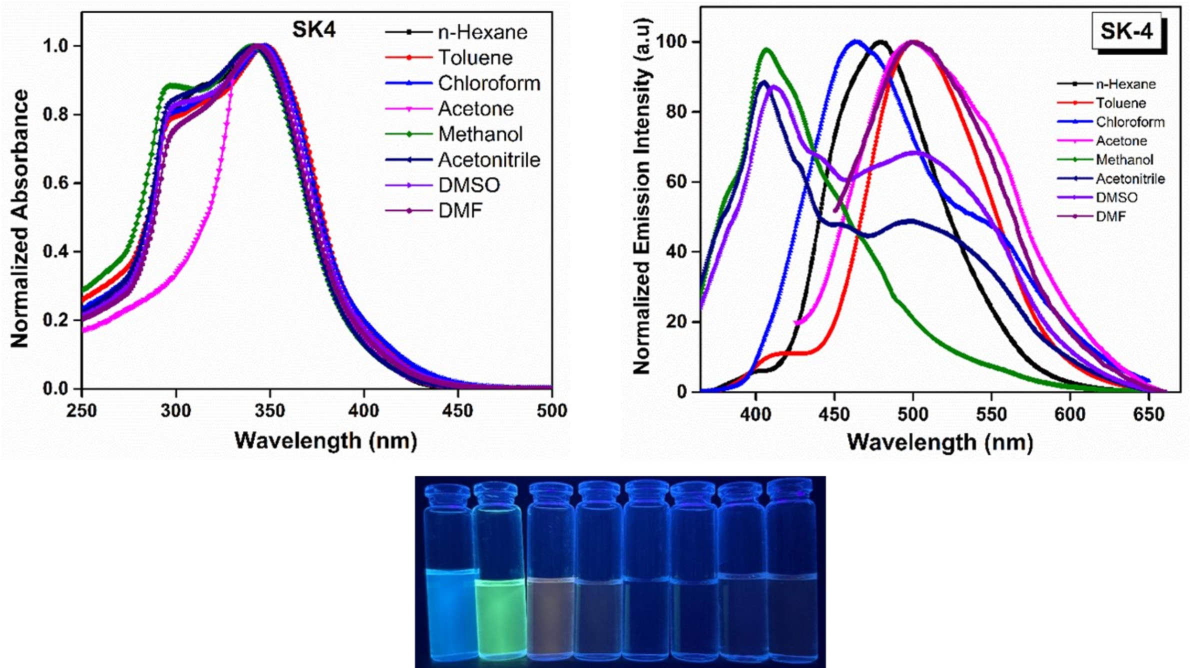


Figure. S9. Absorption, emission spectra of **SK-4** in solvents with graded polarity (From left: *n*-hexane, Toluene, Chloroform, Acetone, Methanol, Acetonitrile, DMSO, DMF).

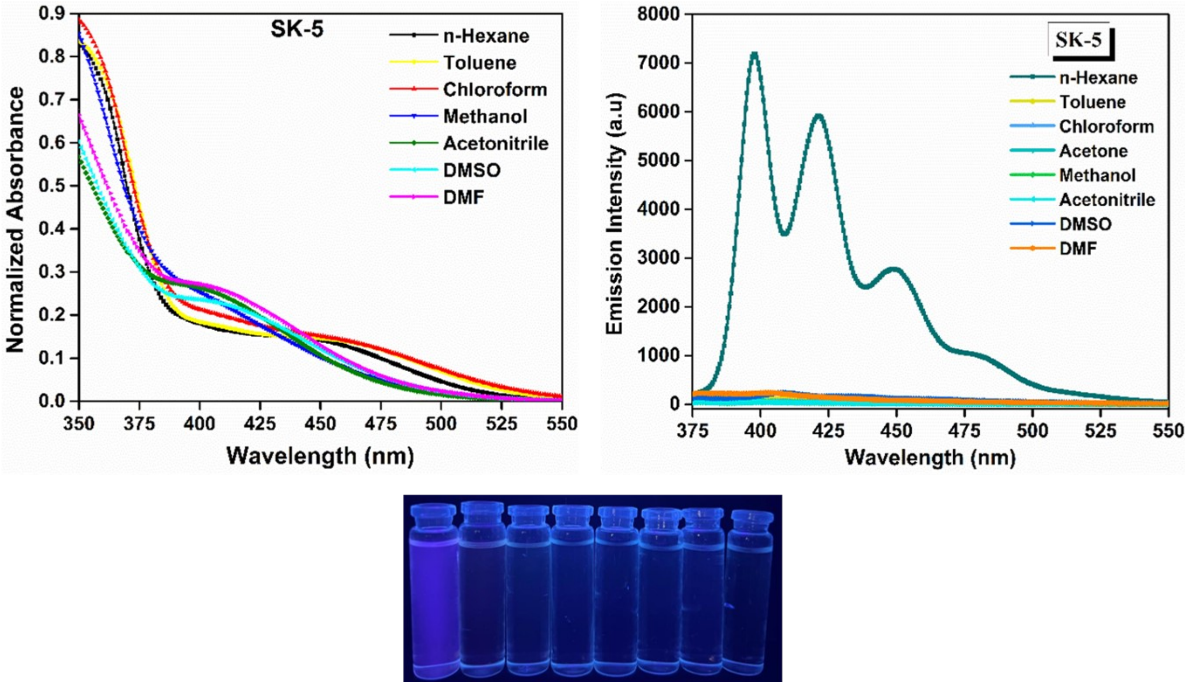


Figure. S10. Absorption, emission spectra of **SK-5** in solvents with graded polarity (From left: *n*-hexane, Toluene, Chloroform, Acetone, Methanol, Acetonitrile, DMSO, DMF).

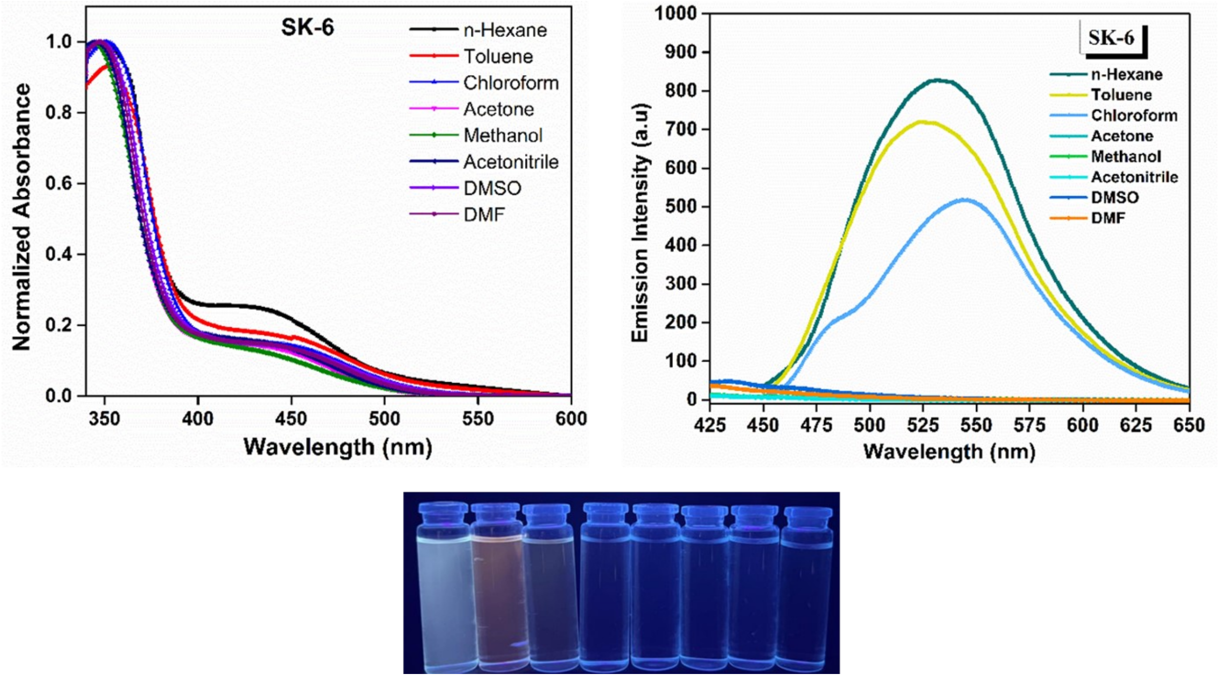


Figure. S11. Absorption, emission spectra of **SK-6** in solvents with graded polarity (From left: *n*-hexane, Toluene, Chloroform, Acetone, Methanol, Acetonitrile, DMSO, DMF).

Aggregation Induced Emission Studies of SK-1 to SK-6

Aggregation-induced emission (AIE) studies were conducted to elucidate the photophysical properties of molecules in suitable solvent of different concentrations with water under varying aggregation and dilution states. All studies were performed using tetrahydrofuran in different concentration with water. The concentration of stock solution of **SK-1 to SK-6** used for studied was 1 mM. Absorption studies performed in JASCO V-750 spectrophotometer under room temperature using two side opaque and two side transparent quartz cuvettes having path length equalled to 1 cm. For photoluminescence studies, the emission measurement was performed in a JASCO FP-8200 spectrofluorometer under room temperature using all side transparent quartz cuvette with path length equal to 1cm.

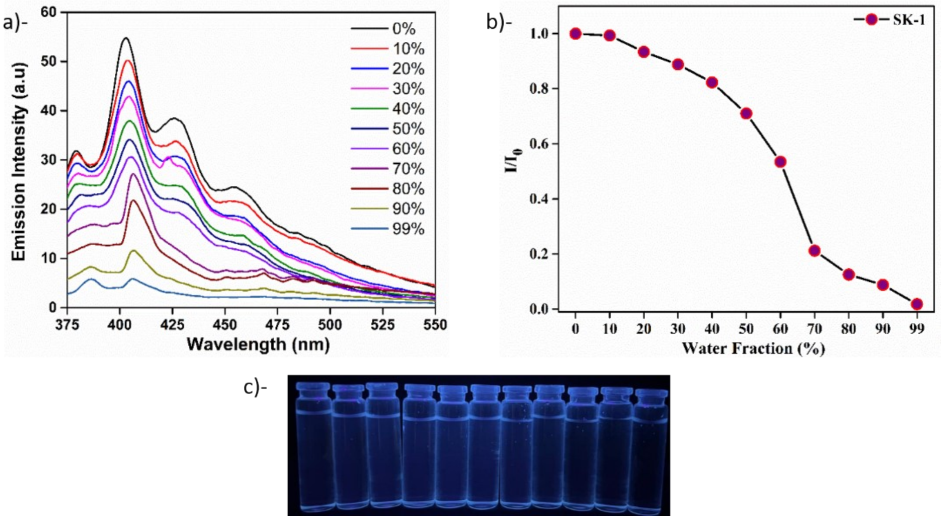


Figure S12. a) AIE emission, b) I/I_0 graph of **SK-1** and c) photographs of vials comprising **SK-1** in different THF/H_2O content (left to right: 0% water to 99% water).

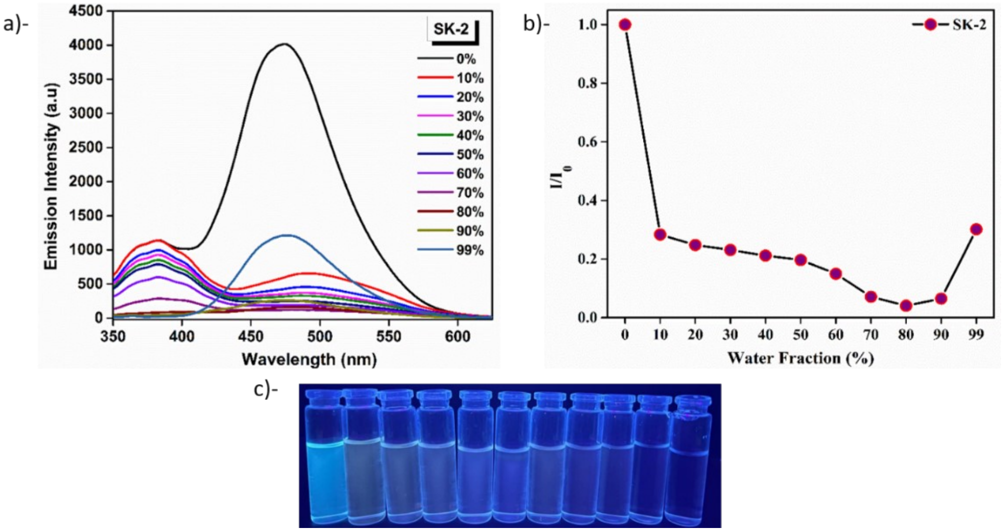


Figure. S13. a) AIE emission, b) I/I_0 graph of **SK-2** and c) photographs of vials comprising **SK-2** in different THF/H_2O content (left to right: 0% water to 99% water).

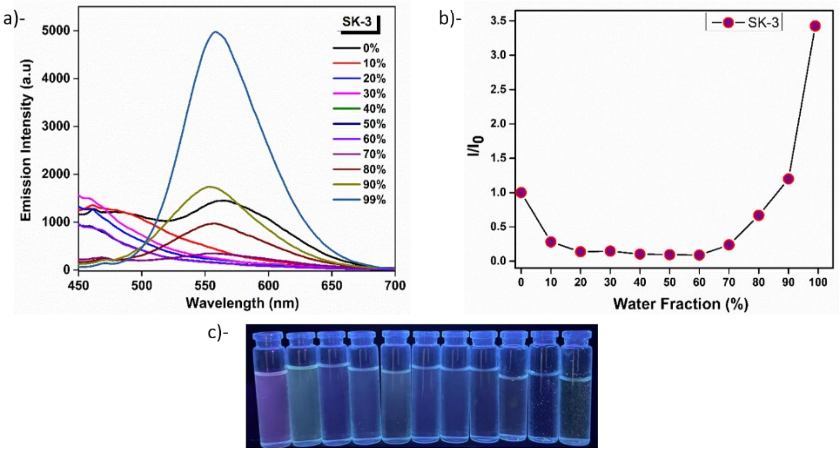


Figure. S14. a) AIE emission, b) I/I$_0$ graph of of **SK-3** and c) photographs of vials comprising **SK-3** in different THF/H$_2$O content (left to right: 0% water to 99% water).

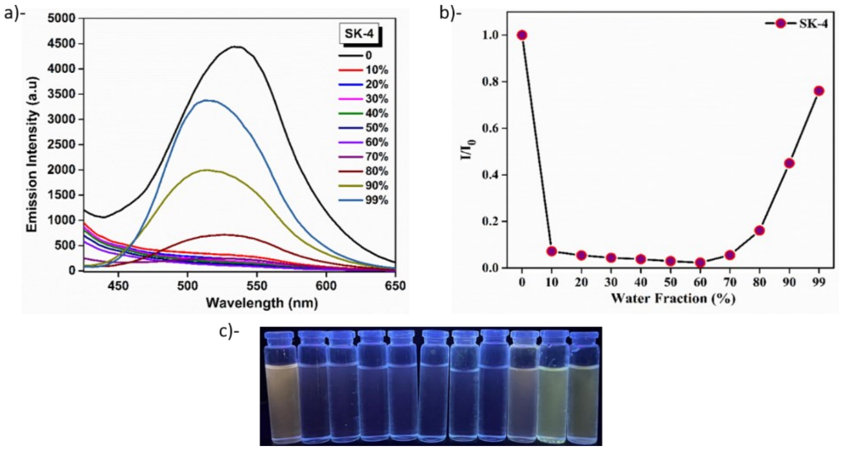


Figure. S15. a) AIE emission, b) I/I$_0$ graph of **SK-4** and c) photographs of vials comprising **SK-4** in different THF/H$_2$O content (left to right: 0% water to 99% water).

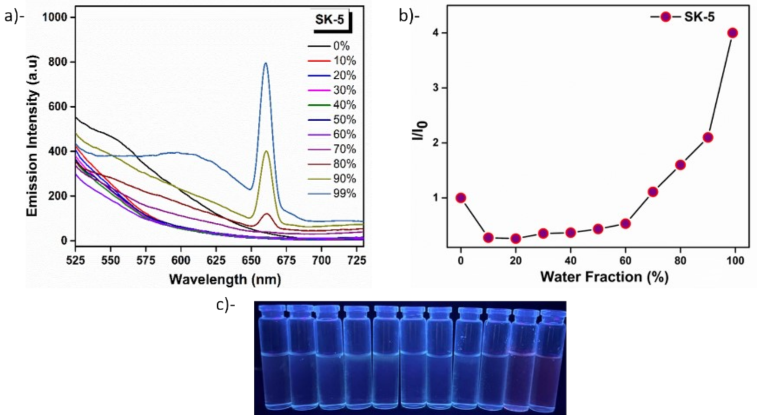


Figure. S16. a) AIE emission, b) I/I$_0$ graph of **SK-5** and c) photographs of vials comprising **SK-5** in different THF/H$_2$O content (left to right: 0% water to 99% water).

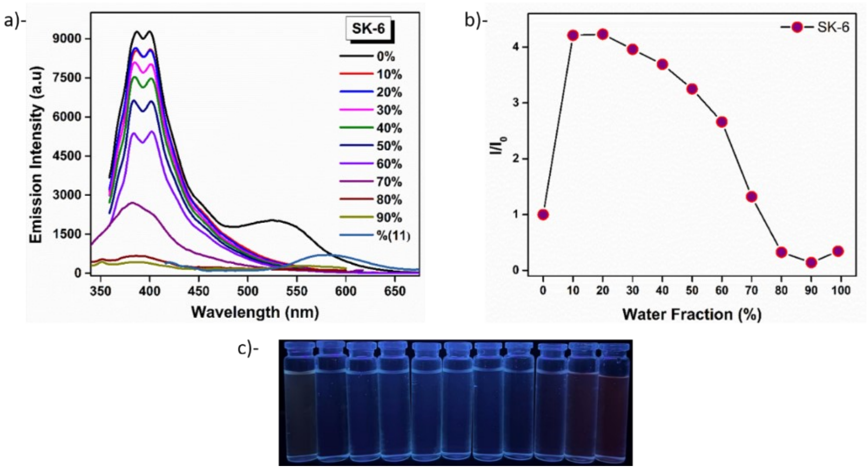


Figure. S17. a) AIE emission, b) I/I_0 graph of of **SK-6** and c) photographs of vials comprising **SK-6** in different THF/H_2O content (left to right: 0% water to 99% water).

Dynamic Light Scattering (DLS) Experiments and Tyndall Effect of SK-2 to SK-6

The size distribution of the evolved aggregates in THF at higher water fraction was determined through a DLS experiment, using the Malvern Zetasizer Nano-ZS90 instrument. A transparent disposable polystyrene cuvette with a path length equal to 1 cm, containing the desired solution was utilized in the experiment. A 632.8 nm red laser was employed as an excitation source at a fixed scattering angle (90˚ optics).

Tyndall effect was studied by passing laser light through the maximum aggregated state and dilution state (100% THF) of luminogens. The solution containing 99% water shows light scattering and make the beam visible which confirms aggregate formation. While in 100% THF solution light pass away without any appearance, that indicates that no aggregates have been formed.

Table S3. DLS parameter of luminogens **SK-2 to SK-6** at their aggregated state having highest emission intensity.

Luminogens	Z-Average (nm)	PDI
SK-2	181.4	0.193
SK-3	491.9	0.608
SK-4	453.2	0.373
SK-5	995.0	0.316
SK-6	412.5	0.151

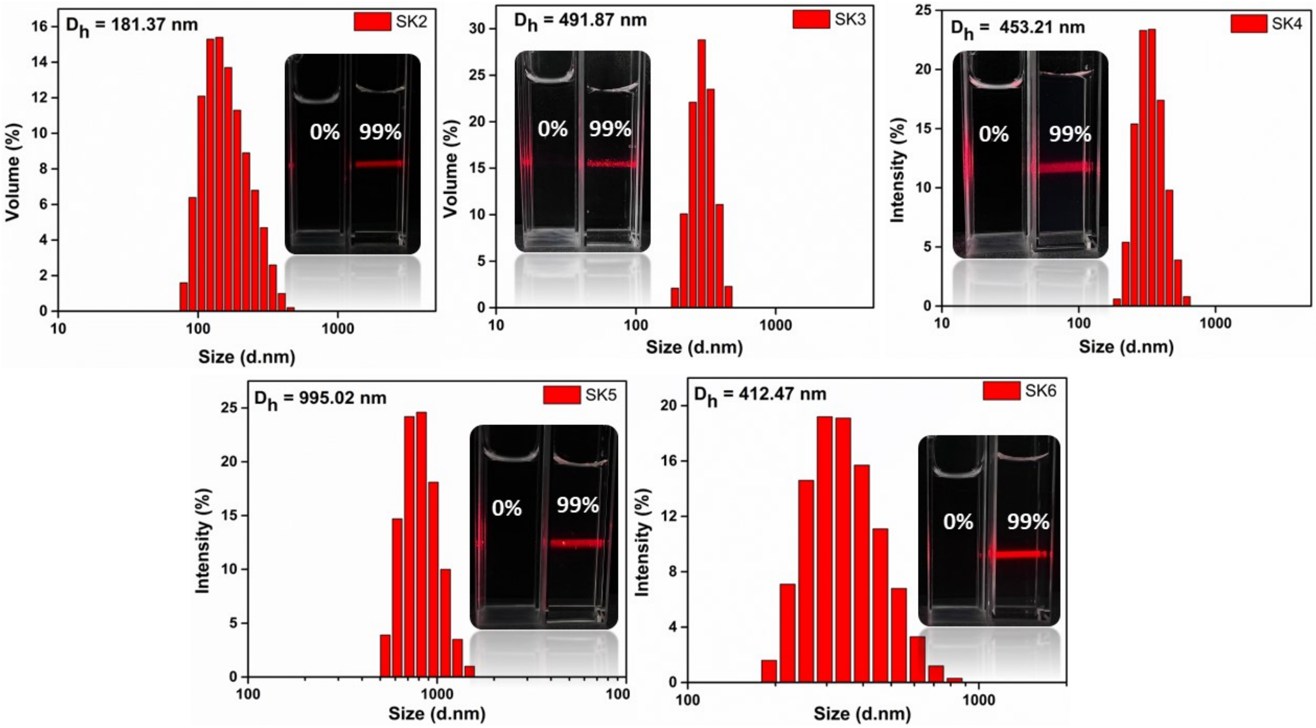


Figure. S18. DLS spectra of **SK-1 to SK-6** at their aggregated states and the inset image shows Tyndall effect (left is 100% THF and right is the aggregated state).

Thermally Activated Delayed Fluorescence Experiment of SK-3 and SK-4

To investigate the TADF process emission spectra of the luminogen **SK-3** and **SK-4** were recorded in 1mM THF solution, were also recorded after degassing the solution by N_2 gas and the significant enhancement of intensity was observed as seen below. The sensitivity of emission intensity towards nitrogen purging i.e. replacement of oxygen with N_2 can be attributed to the involvement of TADF process in these molecules.

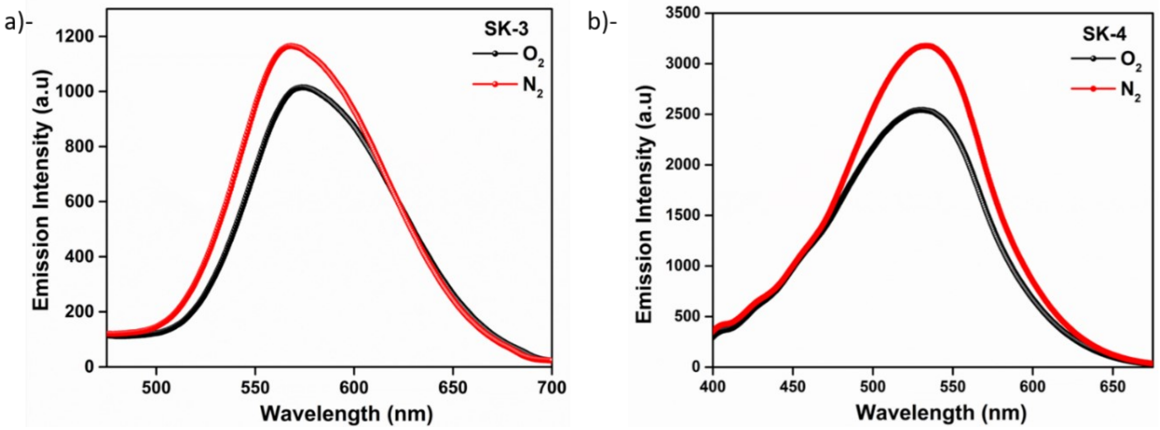


Figure. S19. Emission spectra of a) **SK-3** and b) **SK-4** in aerated solution and nitrogen degassed solution of THF (1mM).

Single Crystal XRD of SK-2 and SK-3

Single Crystal XRD Analysis of SK-2 and SK-3 The Single crystal XRD data has been collected on single crystal X-ray diffractometer of Bruker Smart Apex Duo diffractometer at 100 K using Mo Kα radiation (λ = 0.71073 Å). The frames were integrated with the Bruker SAINT Software package using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The structure was solved and refined using the Bruker SHELXTL Software Package. The structure figure was generated with ORTEP.

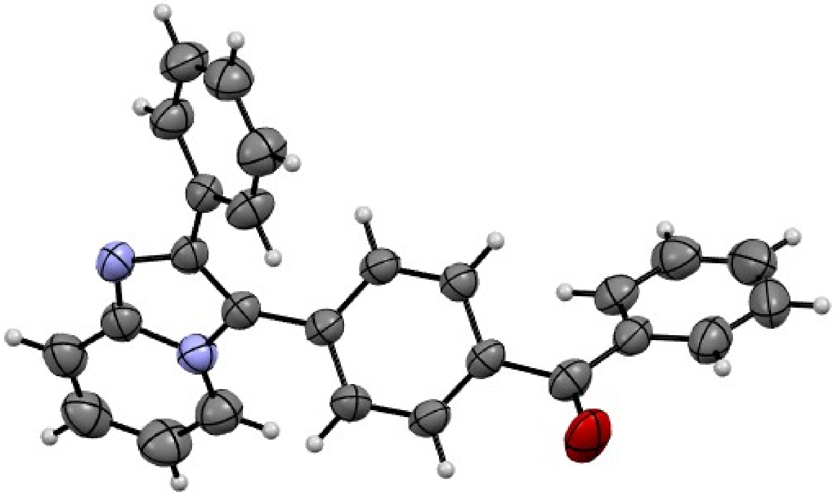


Figure S20. Single crystal data and structure refinement for **SK-2.**

Table S4. Single crystal data and structure refinement for **SK-2.**

Identification code	**SK-2**
Empirical formula	C26 H18 N2 O
Formula weight	374.42
Temperature	298 K
Wavelength	0.71073
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	
a(Å)	8.803 (6)
b(Å)	10.138 (6)

c(Å)	12.016 (8)
α(Å)	101.464 (19)
β(Å)	96.13 (2)
γ(Å)	108.95 (2)
Volume	976.9 (11)
Z	2
Density (calculated)	1.273
Absorption coefficient	0.078
F(000)	392
Refinement method	SHELXL 2017/1 (Sheldrick, 2017)
Goodness-of-fit on F2	0.955

$$R_1 = \frac{\sum \| F_0| - |F_c \|}{\sum |F_0|}$$

$$R_w = \sqrt{\frac{\left[\sum\left\{w\left(F_0^2 - F_c^2\right)^2\right\}\right]}{\left[\sum\left\{w\left(F_0^2\right)^2\right\}\right]}}$$

SK-3

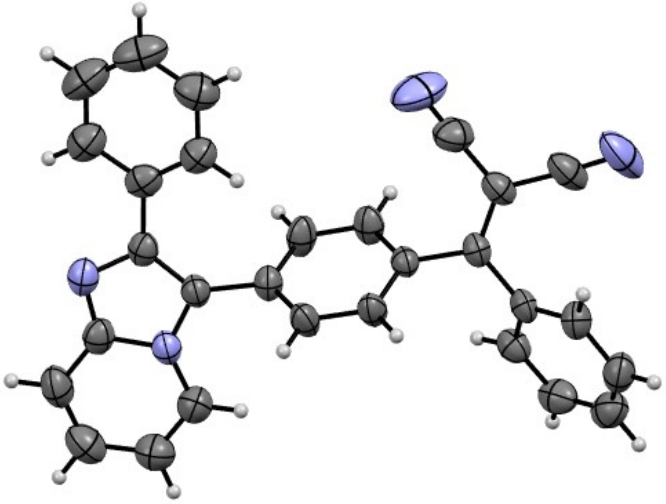


Figure S21. Single crystal data and structure refinement for **SK-3.**

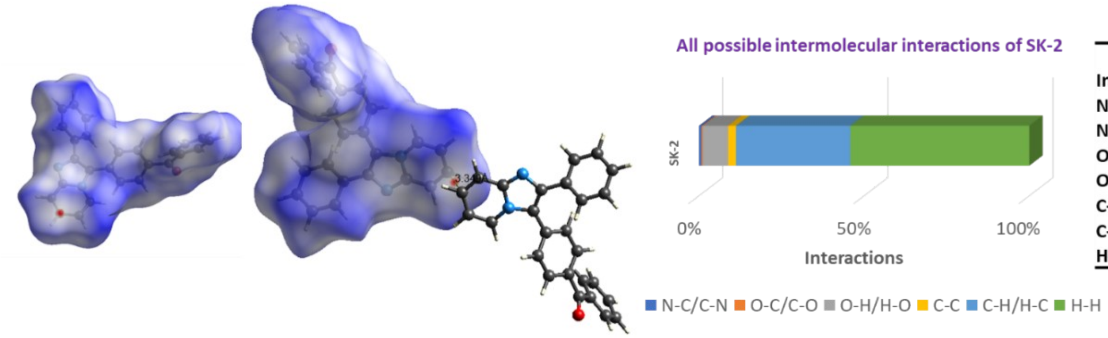
Table S5. Single crystal data and structure refinement for **SK-3**

Identification code	SK-3
Empirical formula	C29 H18 N4
Formula weight	422.47
Temperature	298 K
Wavelength	0.71073
Crystal system	monoclinic
Space group	P 1 21 1
Unit cell dimensions	
a(Å)	11.4434(18)
b(Å)	8.0778(13)
c(Å)	12.613(2)
α(Å)	90
β(Å)	106.227(4)
γ(Å)	90
Volume	1119.4(3)
Z	2
Density (calculated)	1.253
Absorption coefficient	0.076
F(000)	440
Refinement method	SHELXL 2017/1 (Sheldrick, 2017)
Goodness-of-fit on F2	0.848

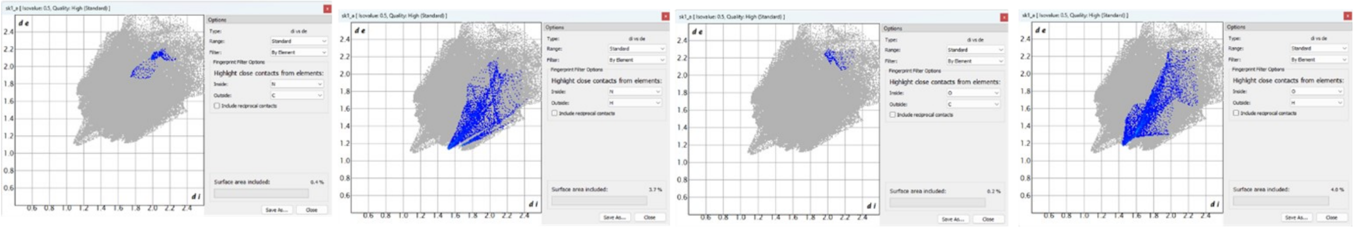
$$R_1 = \frac{\sum \| F_0| - |F_c \|}{\sum |F_0|}$$

$$R_w = \sqrt{\frac{\left[\sum\left\{w\left(F_0^2 - F_c^2\right)^2\right\}\right]}{\left[\sum\left\{w\left(F_0^2\right)^2\right\}\right]}}$$

Heirschfield Surface Analysis



Interactions	% Contribution
N-H	3.7
N-C/C-N	0.8
O-C/C-O	0.4
O-H/H-O	7.3
C-C	2.3
C-H/H-C	33.3
H-H	52.2

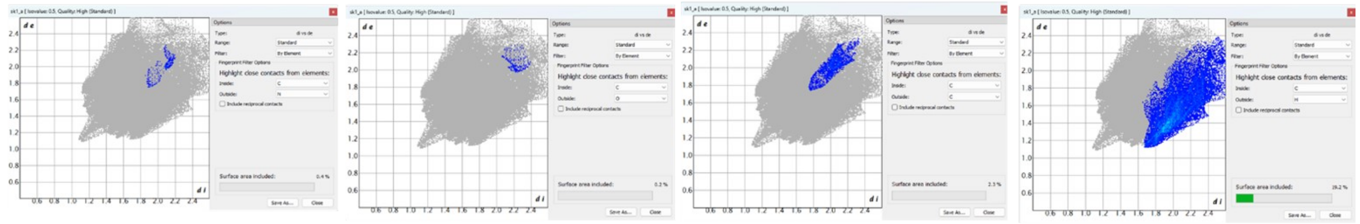


N-C interactions: 0.4%

N-H interactions: 3.7%

O-C interactions: 0.2%

O-H interactions: 4.0%

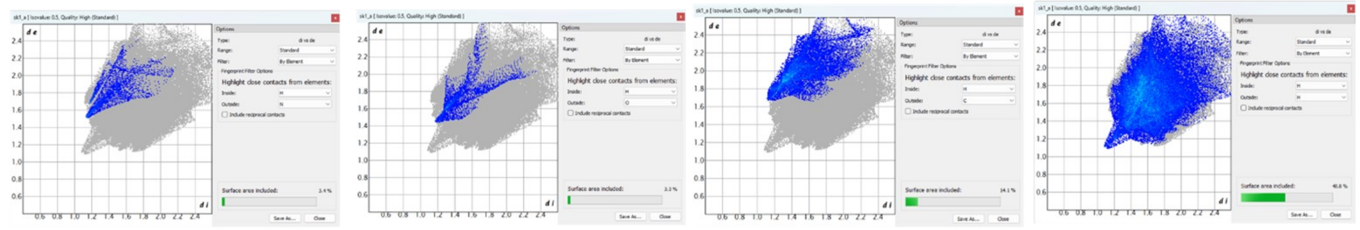


C-N interactions: 0.4%

C-O interactions: 0.2%

C-C interactions: 2.3%

C-H interactions: 19.2%



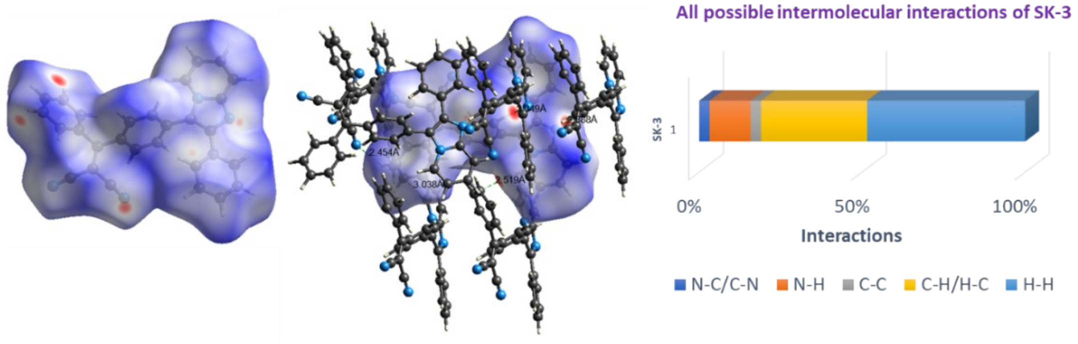
H-H interactions: 3.4%

H-O interactions: 3.3%

H-C interactions: 14.1%

H-H interactions: 48.8%

Figure. S22. Hirschfield surface energy plot and finger plots showing different interactions within the crystal lattice of **SK-2** using Crystal Field Explorer.



Interactions	% Contribution
N-C/C-N	3.2
N-H	12.5
C-C	3.2
C-H/H-C	32.4
H-H	48.3

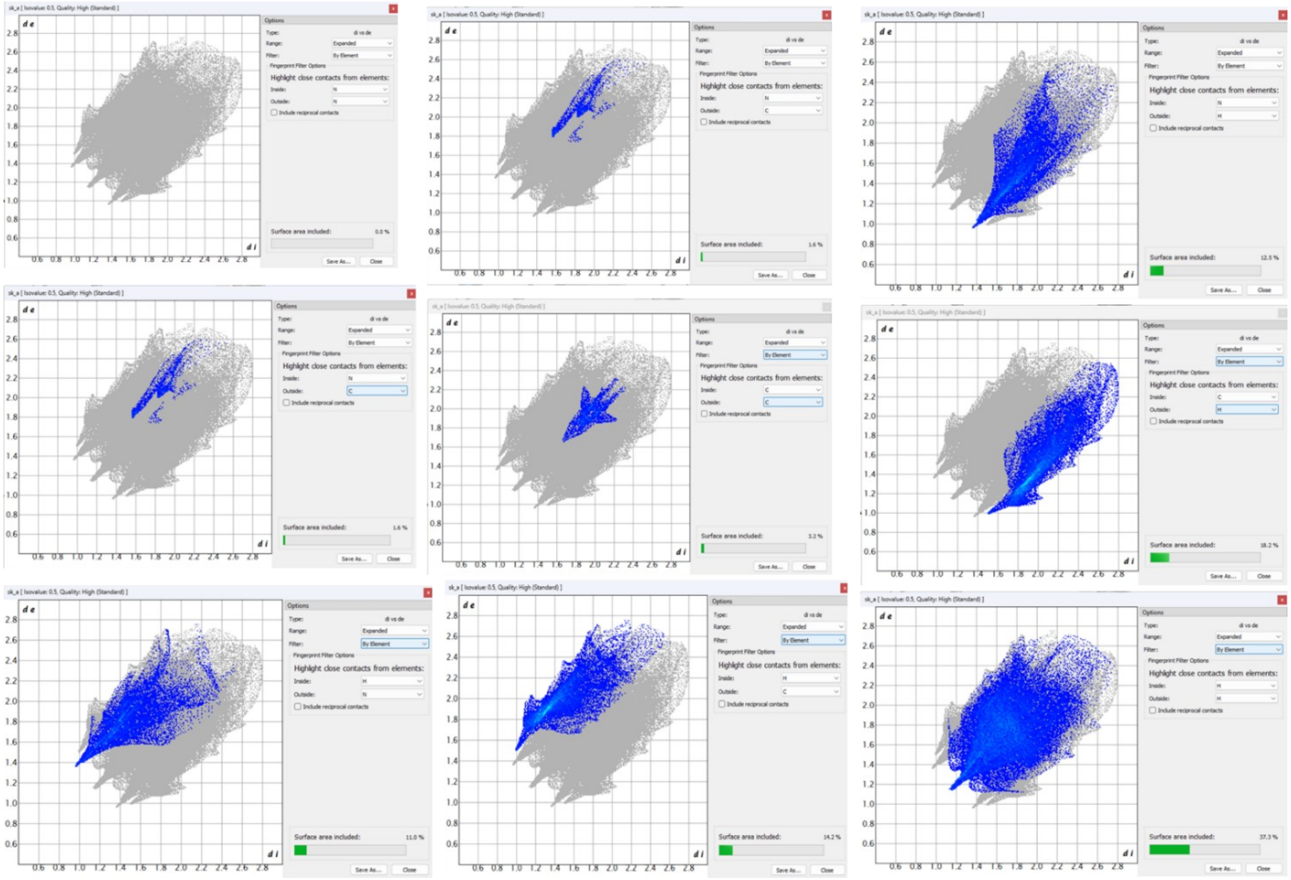


Figure S23. Hirschfield surface energy plot and finger plots showing different interactions within the crystal lattice of **SK-3** using Crystal Field Explorer.

Photostability Studies of SK-2 to SK-6

Photostability is a crucial parameter for fluorescent probes, as it directly impacts their reliability and performance in both fluorescence detection and imaging applications. To study the effect of UV light on the luminogens we carried out its photostability analysis. 1mM solution was prepared of all the luminogens (except for SK-1 which is non-emissive in nature). These solutions were then subjected UV radiation for 30 minutes and their fluorescence emission was recorded with spectrofluorometer at every 5 min interval up to 30 minutes. As reflected in table S24 all the luminogens show good stability towards UV light and are stable. 32% quenching is seen in SK-2 and SK-4 whereas compound SK-6 shows 25% quenching as compared to its initial emission intensity. SK-3 and SK-5 show least quenching and are found to be stable towards UV light exposure for 30 minutes with minimal quenching percentage of 12% and 8.5% respectively. These data confirm that our probes exhibit good photostability and show minimum photobleaching effect.

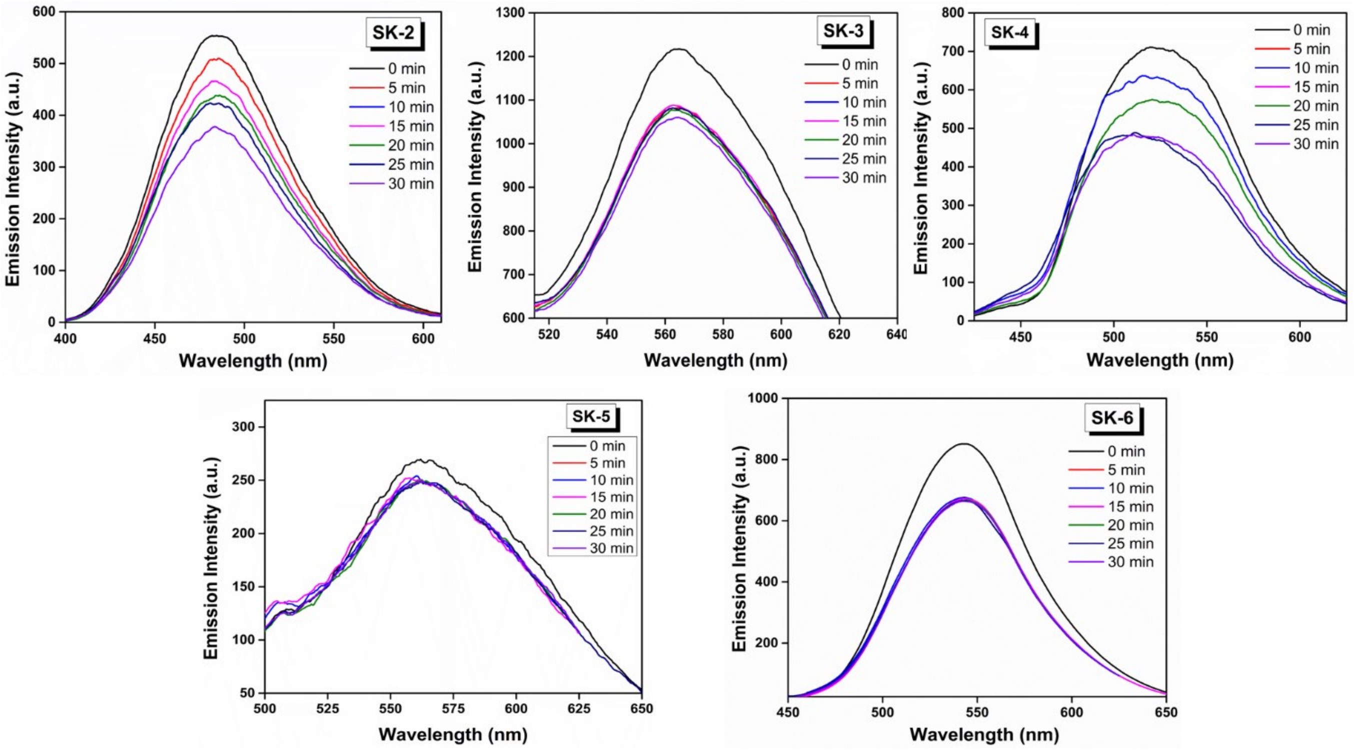


Figure S24. Photostability graphs of **SK-2** to **SK-6** showing changes in emission intensity after exposure of UV light from 0 minute to 30 minutes.

Table S6. Table showing percentage quenching of luminogens **SK-2** to **SK-6** after exposure of UV light from 0 minute to 30 minutes.

Luminogens	Quenching (%)
SK-2	32
SK-3	12
SK-4	32
SK-5	8.5
SK-6	25

Bio-imaging Studies of SK-3, SK-4 and SK-6

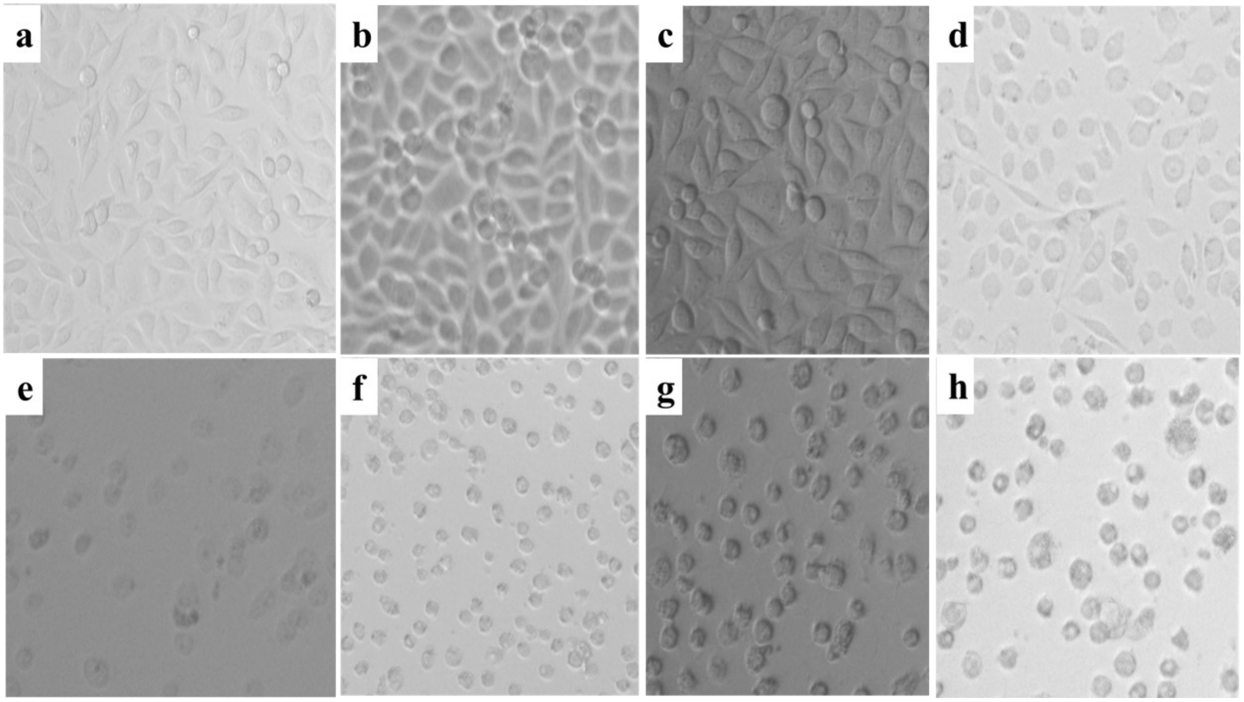


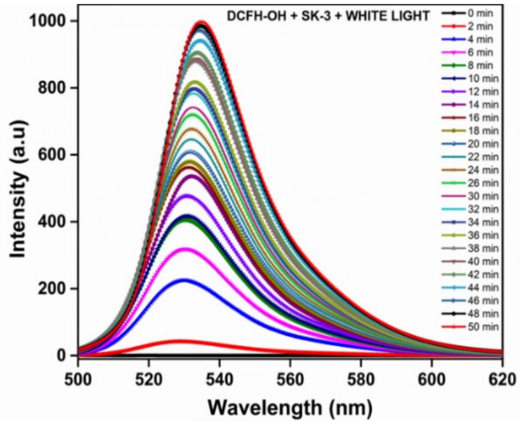
Figure. S25. Two-dimensional images depicting inhibition of SiHa cell growth after 24-hour incubation with luminogens **a)** and **e)** represent growth control and positive control, respectively; **b)** and **f)** cells treated with 0.1 µg/ml and 1 µg/ml concentration of **SK-3**; **c)** and **g)** represent cells treated with 0.1 µg/ml and 1 µg/ml concentration of **SK-4**; **d)** and **h)** represent cells treated with 0.1 µg/ml and 1 µg/ml concentration of **SK-6**.

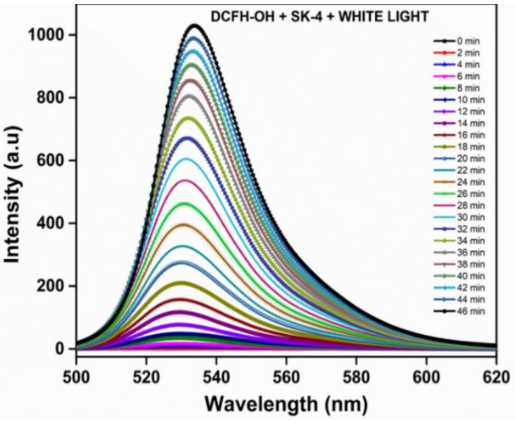
Reactive Oxygen Species Experimental Details for SK-3, SK-4 and SK-6

DCFH-DA (1mM, 5 mL) stock solution was made in dry ethanol and used for the study. 3 mL of dry ethanol was taken in a cuvette to which DCFH-DA (120 µl) was added from stock solution of 1mM resulting in 40 µM of DCFH-DA solution. To this solution was added 120 µl of NaOH solution of 40 µM concentration. This solution was subjected to ultrasonication under dark conditions for 15 minutes to form DCFH-OH. Luminogen (60 µl, 40 µM concentration) was added to the above solution.

The solution was covered and kept in dark throughout the study. After mixing thoroughly the solution was subjected to white light followed by recording the fluorescence spectra at every 2-minute interval by using an excitation wavelength of DCFH-DA of 504 nm and emission was recorded at 530 nm.

The above procedure was followed for blank without the addition of the luminogen. It was observed that DCFH-OH solution which was kept in dark gave only marginal fluorescence enhancement over 40 minutes. However, the DCFH-OH solution which was subjected to white light showed an increase in fluorescence intensity of around ~8 times. It is evident from the graph of ROS that luminogen **SK-3, SK-4, SK-6** were responsible in generating the reactive oxygen species. This was evident from enhancement of emission intensity showcased in Fig after subjecting it to white light. Enhancement factor was 7 times, 2 times and 5 times for **SK-3, SK-4, SK-6** respectively when compared to DCFH-OH solution irradiated with white light.





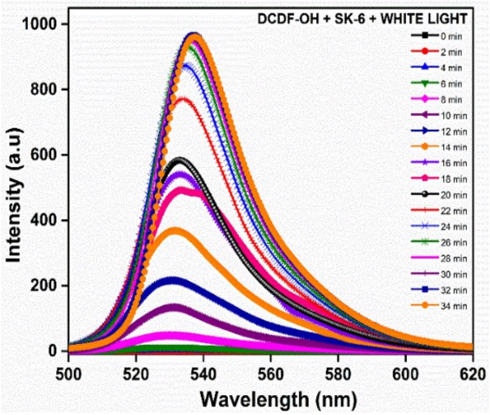


Figure. S26. Fluorescence emission spectra of **SK-3, SK-4** and **SK-6** in presence of DCFH-DA after subjecting to white light at every 2 min interval.

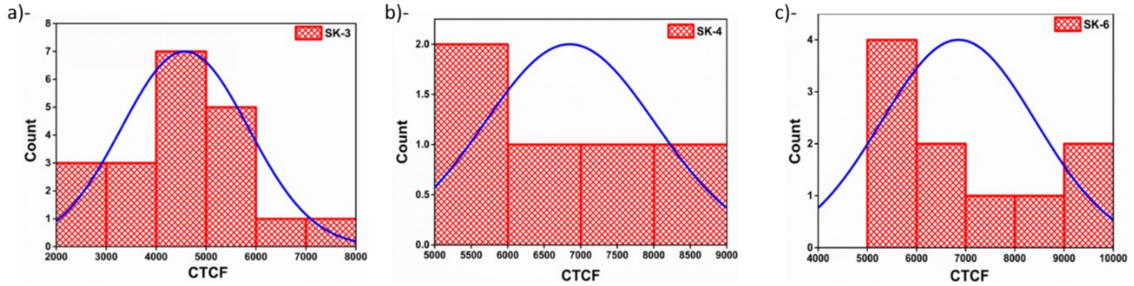
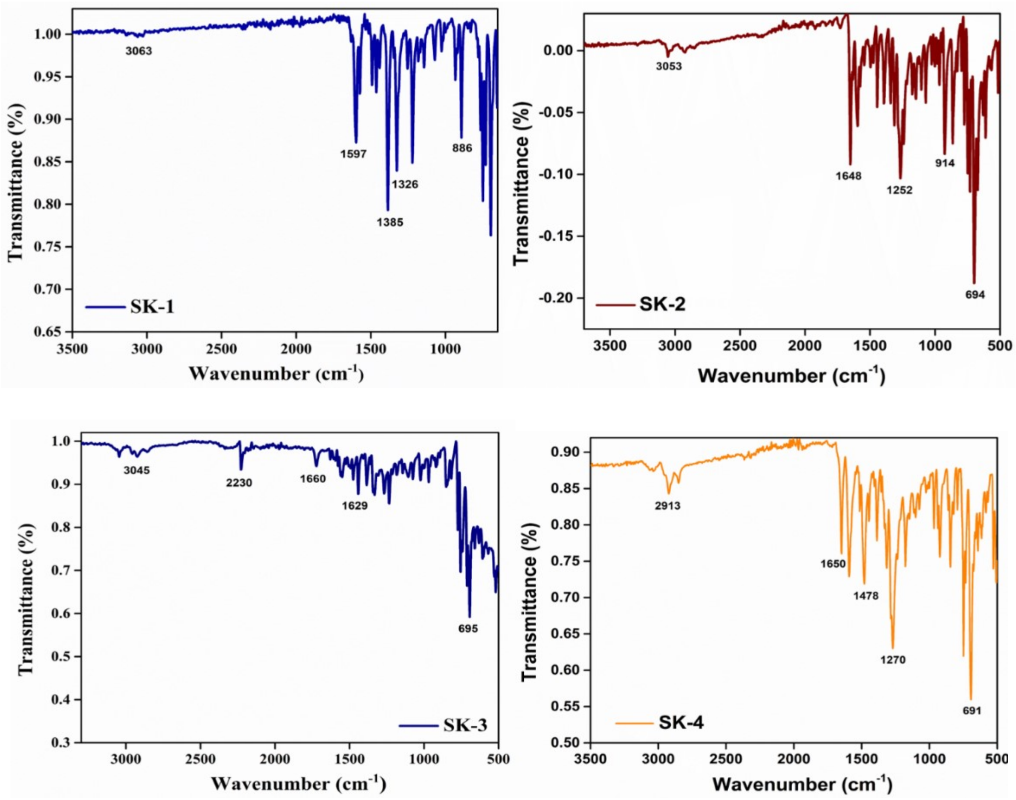


Figure. S27. Fluorescence intensity comparison of **SK-3, SK-4,** and **SK-6.**

IR Spectral Reproductions of SK-1 to SK-6



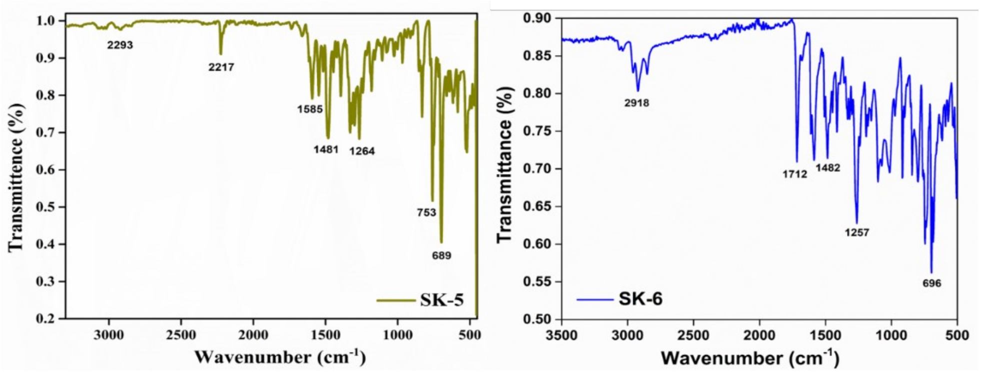


Figure. S28. IR spectra of compounds **SK-1** to **SK-3** (top row) and **SK-4** to **SK-6** (bottom row).

^{1}H and ^{13}C NMR Spectral Representations of SK-1 to SK-6

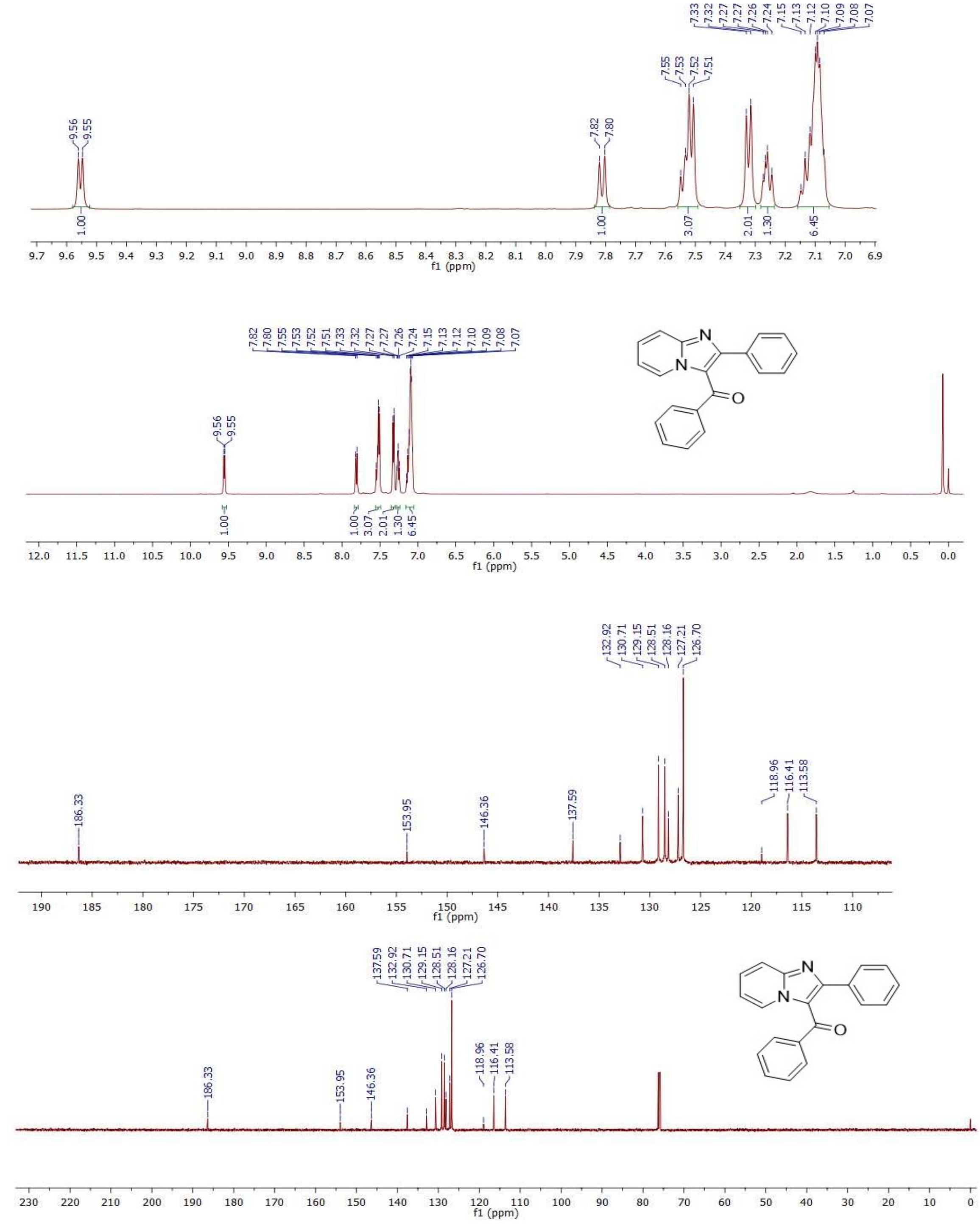


Figure. S29. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (126 MHz, $CDCl_3$) spectra of phenyl(2-phenylimidazo[1,2-a]pyridin-3-yl)methanone **SK-1.**

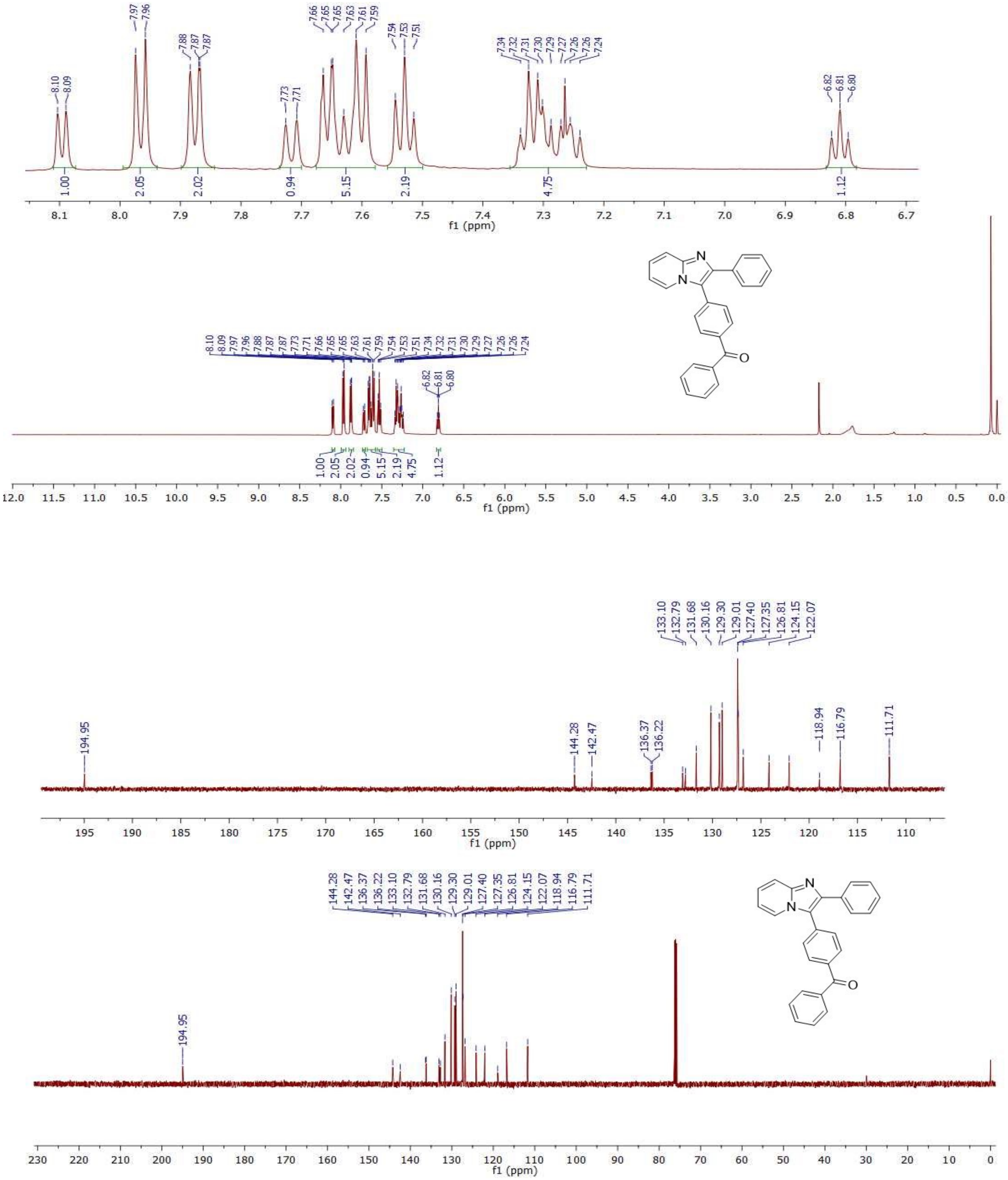


Figure. S30. ^{1}H NMR (500 MHz, CDCl$_3$) and ^{13}C NMR (126 MHz, CDCl$_3$) spectra of phenyl (4-(2-phenyl imidazo (1,2-a) pyridine-3-yl)phenyl)methanone **SK-2.**

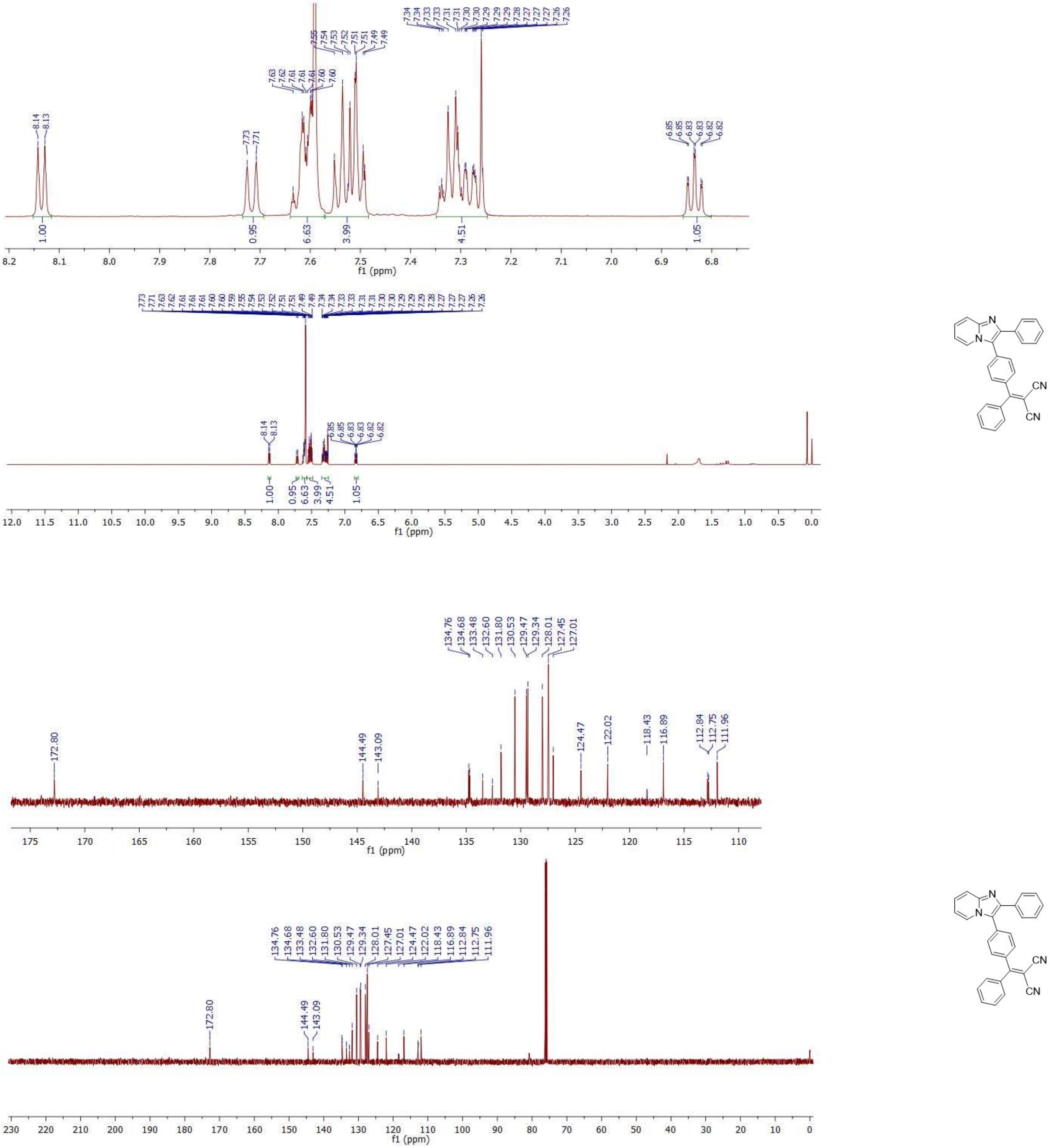


Figure. S31. ^{1}H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (126 MHz, $CDCl_3$) spectra of phenyl (4-(2-phenylimidazo (1,2-a) pyridine-3-yl)phenyl)methylene) malononitrile **SK-3.**

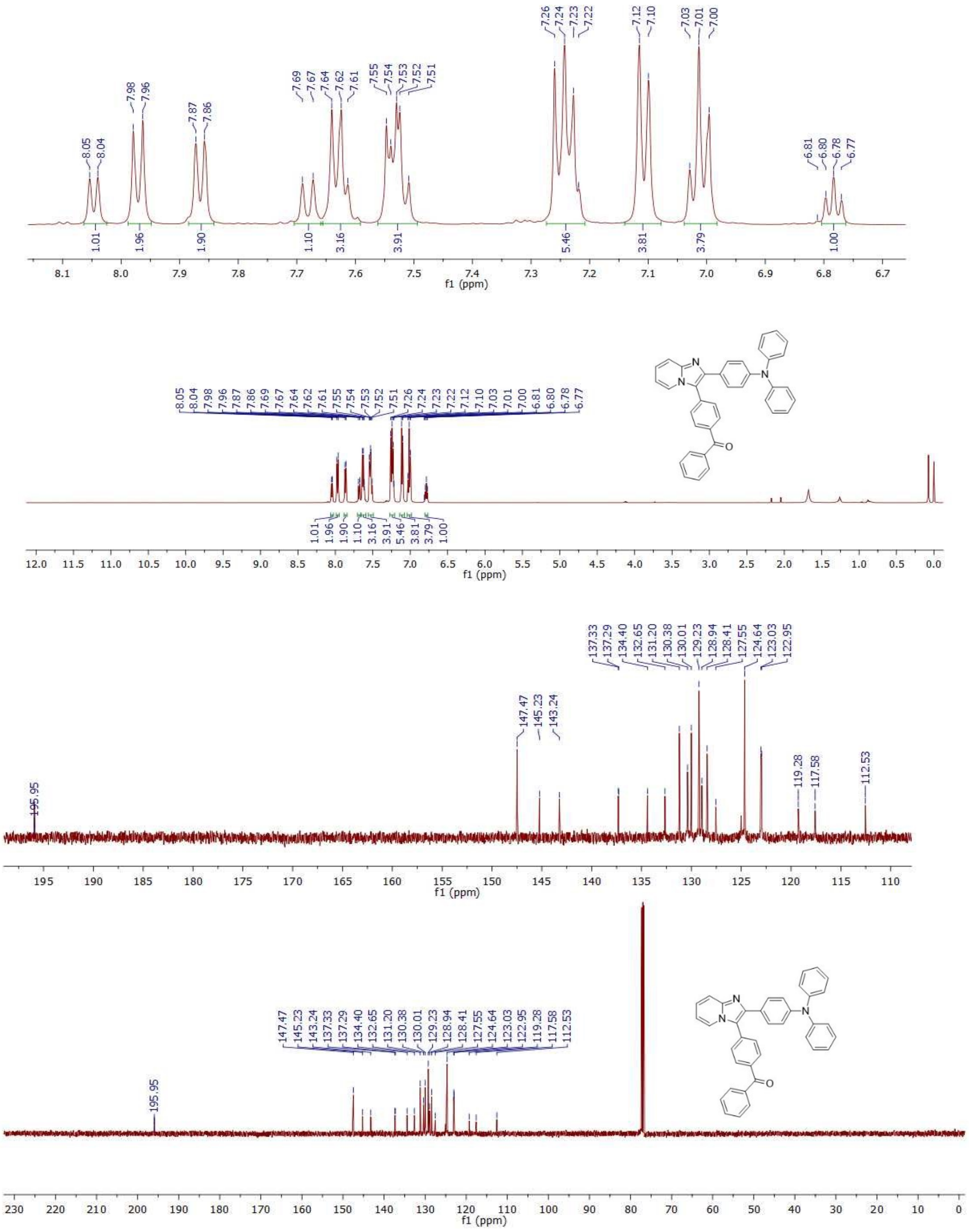


Figure. S32. ^{1}H NMR (500 MHz, CDCl$_3$) and ^{13}C NMR (126 MHz, CDCl$_3$) spectra of (4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methanone **SK-4.**

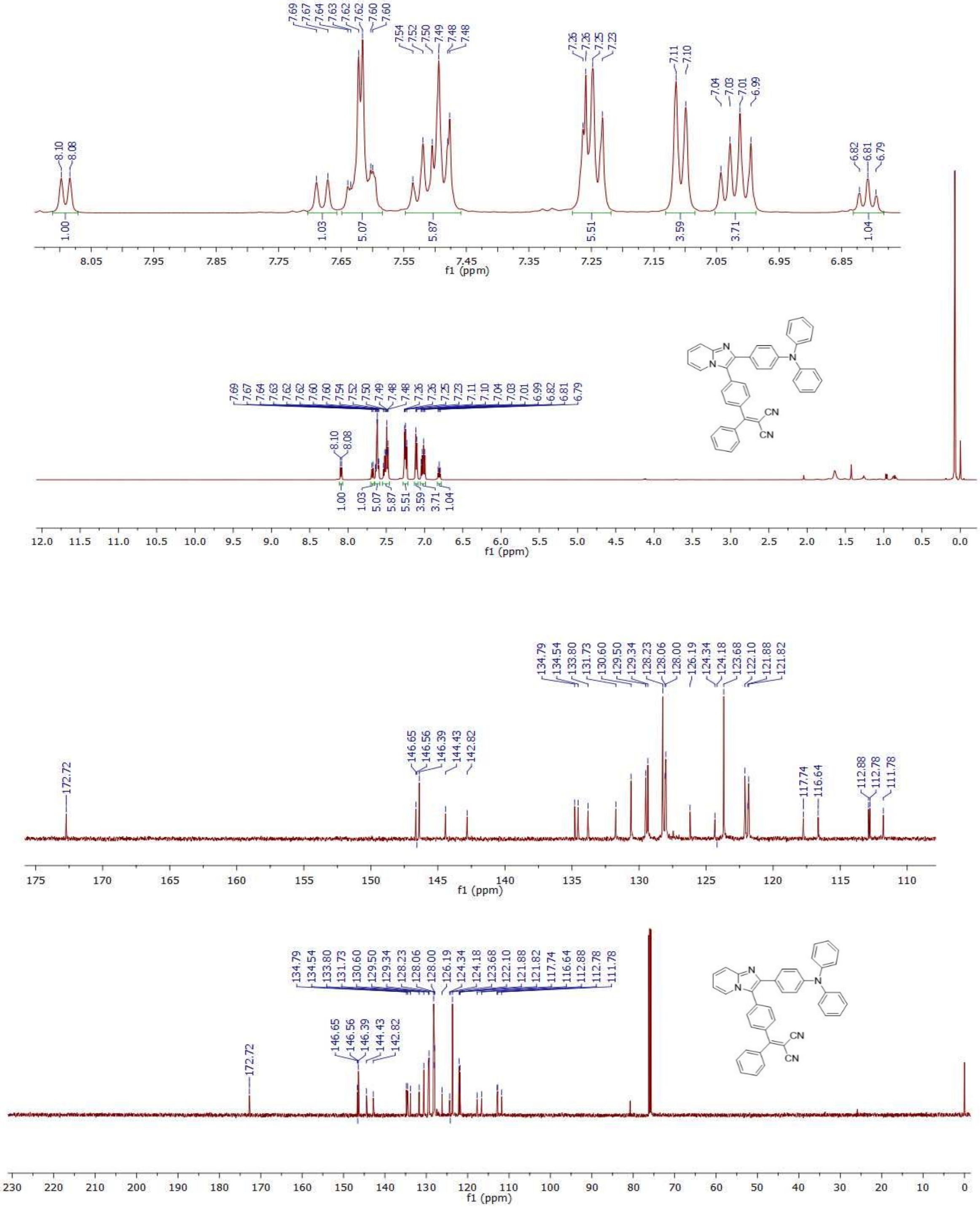


Figure. S33. ^1H NMR (500 MHz, $CDCl_3$) and ^{13}C NMR (126 MHz, $CDCl_3$) spectra of 2-((4(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methylene)malononitrile **SK-5.**

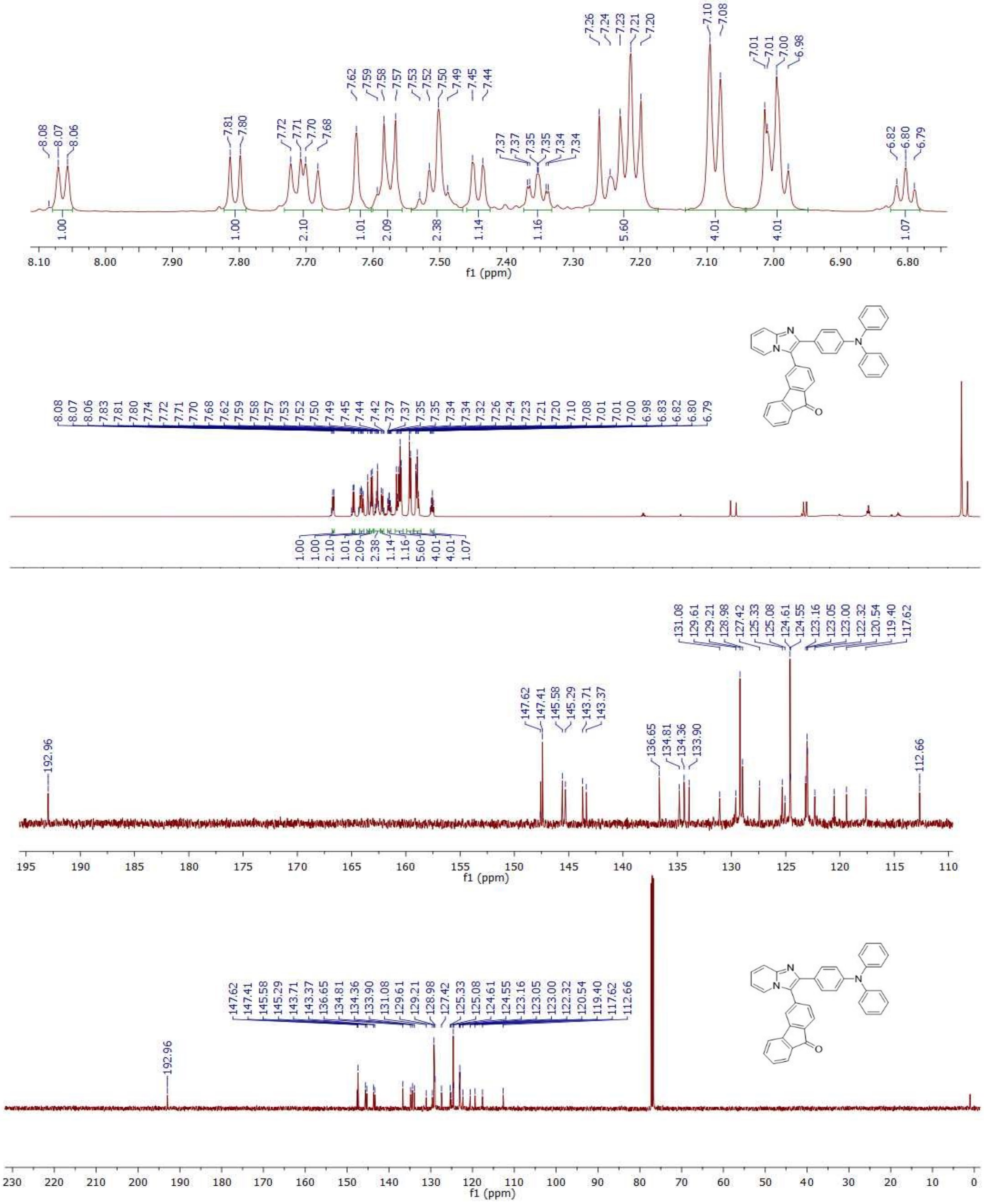


Figure. S34. ^{1}H NMR (500 MHz, CDCl$_3$) and ^{13}C NMR (126 MHz, CDCl$_3$) spectra of 3-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)-9H-fluoren-9-one **SK-6.**

LC-HRMS Data of SK-1 to SK-6

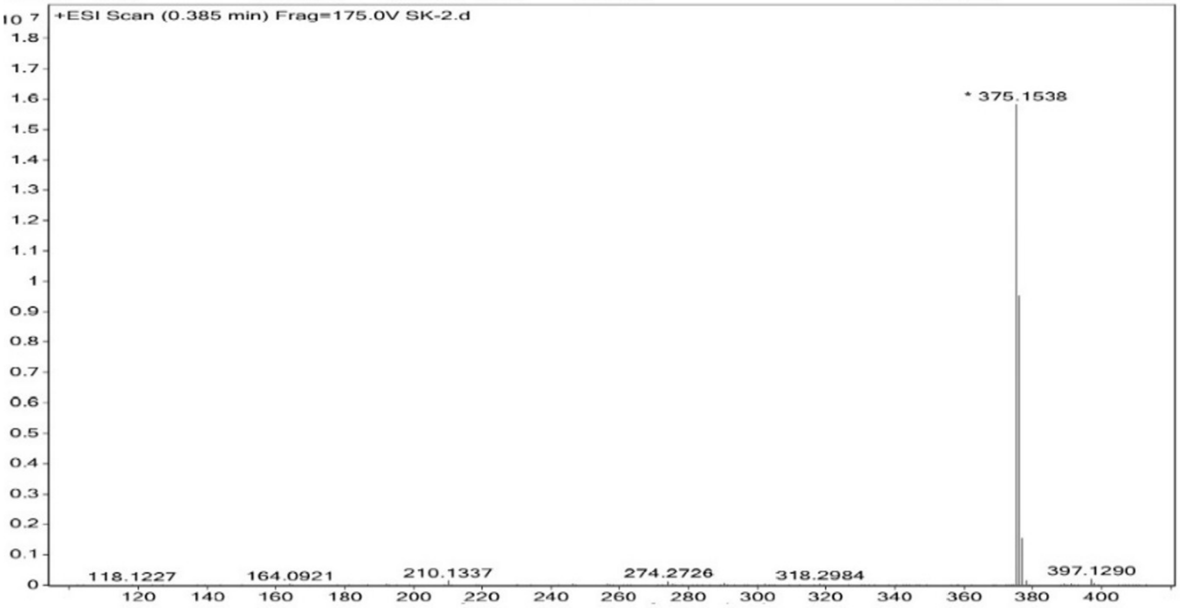


Figure. S35. LC-HRMS spectra of phenyl (4-(2-phenyl imidazo (1,2-a) pyridine-3-yl)phenyl) methanone **SK-2.**

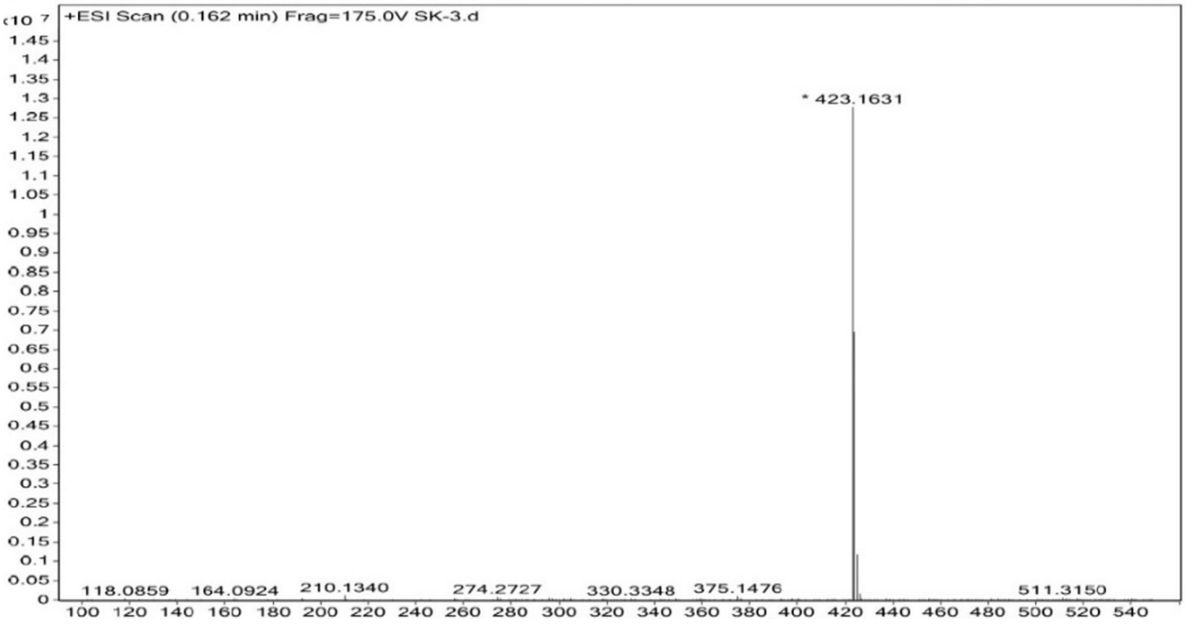


Figure. S36. LC-HRMS spectra of phenyl (4-(2-phenylimidazo (1,2-a) pyridine-3-yl)phenyl)methylene)malononitrile **SK-3.**

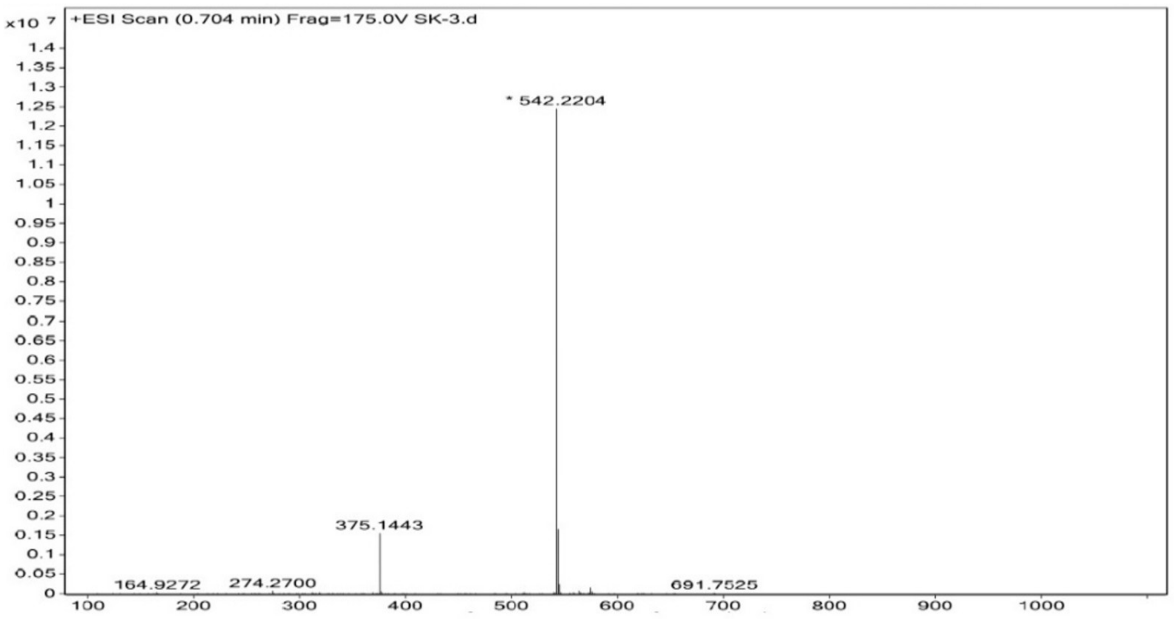


Figure. S37. LC-HRMS spectra of (4-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methanone **SK-4.**

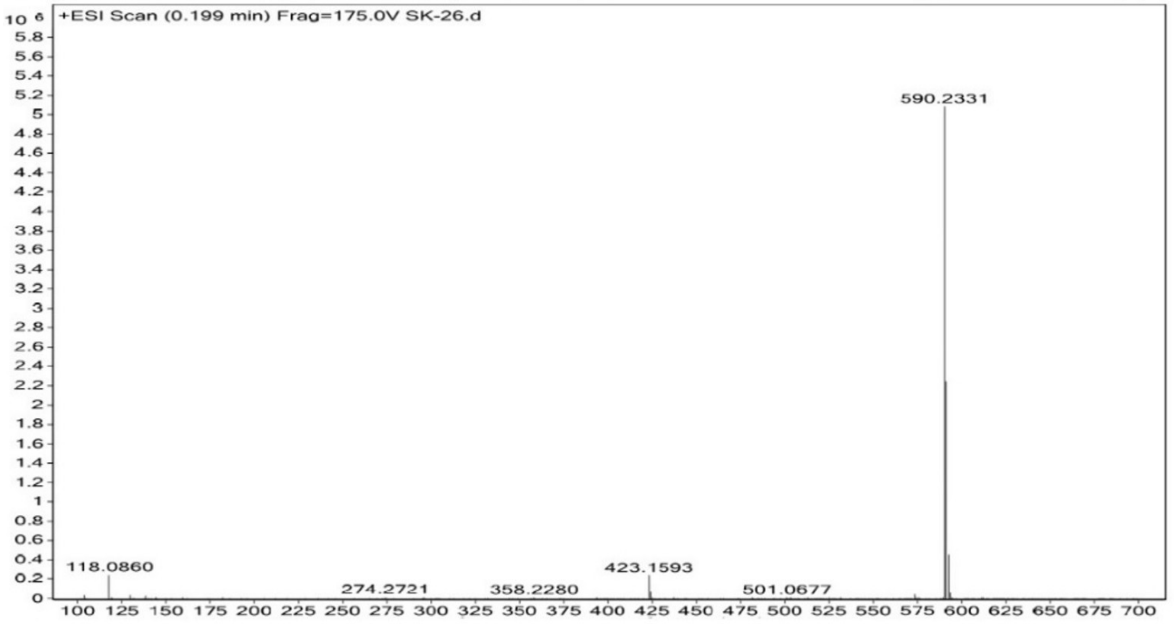


Figure. S38. LC-HRMS spectra of 2-((4(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)phenyl)(phenyl)methylene)malononitrile **SK-5.**

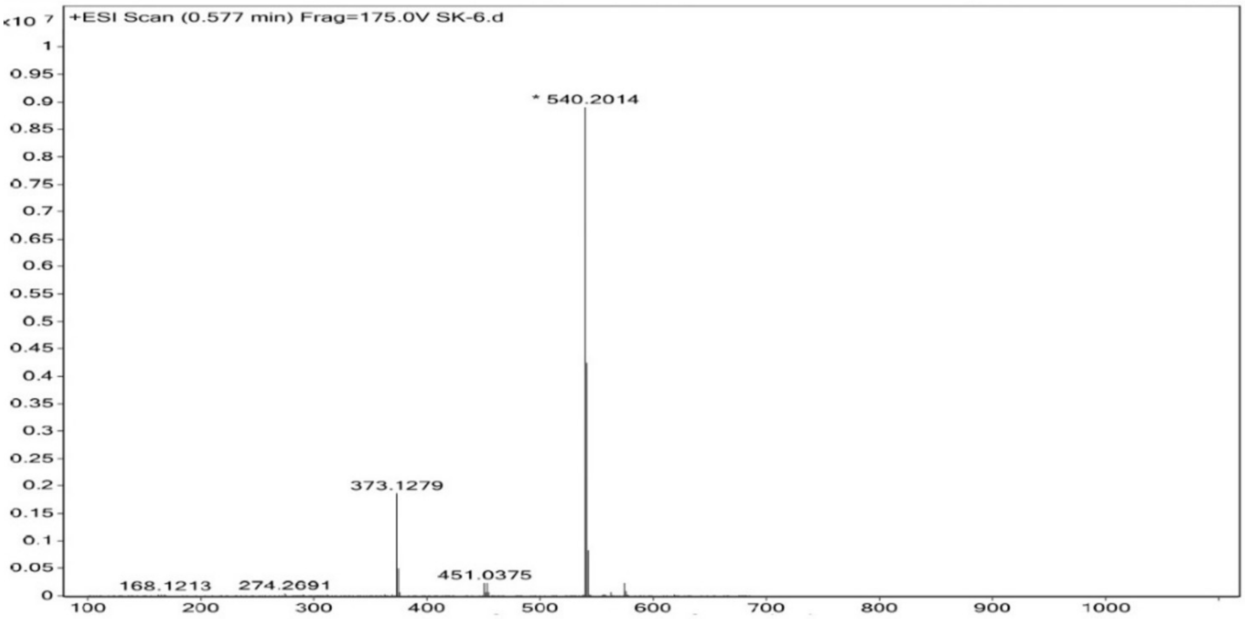


Figure. S39. LC-HRMS spectra of 3-(2-(4-(diphenylamino)phenyl)imidazo[1,2-a]pyridin-3-yl)-9H-fluoren-9-one **SK-6.**

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2. G. Yashwantrao, V. Naik, P. Badani, S. Saha, *Chem. Eur. J.*, 2025, 31, e202500047.
3. J. Issac, S. Ravi, K. Chidambaranathan, S. Karthikeyan, M. Pannipara, A. G. Al-Sehemi, S. P. Anthony, V. Madhu Cryst. Growth Des. 2024, 24, 3388–3398