Supplementary Information

New Indolo Carbazole Based Non-Fullerene n-Type Semiconductors for Organic Solar Cell Applications

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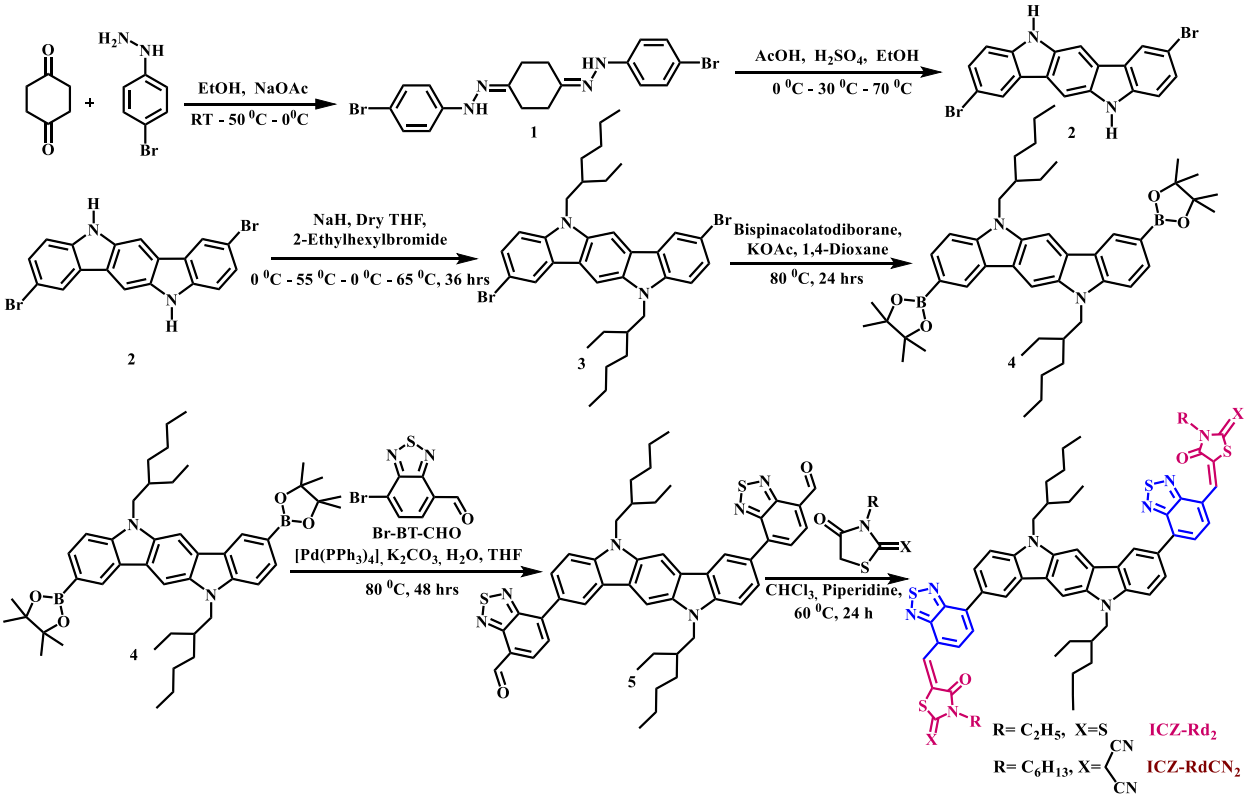
Experimental Section

Materials and Synthesis: All reagents and chemicals were purchased from commercial suppliers and used as received. Anhydrous solvent were dried and purified by distillation over calcium

hydride under nitrogen atmosphere. Reactions were carried out in a nitrogen atmosphere unless otherwise stated. All products were purified using standard flash column chromatography technique on silica gel (60-120 mesh and 100-200 mesh).

Synthetic Procedure:7-bromobenzo[*c*][1,2,5]-thiadiazole-4-carbaldehyde (Br-BT-CHO) and dicyano-n-hexylrhodanine were synthesized according to previous reported procedures.[1-2]



Scheme S1: Synthesis of compound **ICz-Rd$_2$**and**ICz-RdCN$_2$.**

Synthesis of Compound 1:

To a 250 mL round bottom flask 4-bromophenylhydrazine hydrochloride (15.92 g, 17.83 mmol) and sodium acetate (1.64 g, 17.83 mmol) were dissolved in absolute ethanol (100 mL) at room temperature. A solution of 1,4-Cyclohexanedione (4 g, 35.62 mmol) also dissolved in absolute ethanol (50 mL) and added slowly drop wise. After complete addition the reaction mixture was heated to 50 ^{o}C and stirred for 2 hrs. Then the mixture was cooled to room temperature and poured in to ice water with stirring. The precipitate was filtered off and washed carefully with water to yield compound **1** as light yellow solid in 51% yield (8.2 g, 18.21 mmol). ^{1}H NMR (500 MHz,

$CDCl_3$), δ ppm: 7.34-7.31 (d,J=9.00Hz,4H), 6.94-6.92 (d, J=8.85Hz, 4H), 6.90-6.86 (s, 2H) 2.79-2.74 (t, J=6.72Hz, 4H), 2.55-2.50 (t, J=6.86Hz, 4H). ^{13}C NMR (125.77 MHz, $CDCl_3$), δ ppm: 208.34, 132.54, 131.50, 129.90, 124.39, 122.48, 36.68, 27.65, 18.40.

Synthesis of Compound 2:

Compound **1** (8.0 g, 17.77 mmol) was added to a mixture of AcOH (80 mL) and H_2SO_4 (20 mL) in 250 mL round bottom flask at 0 ^{o}C and stirred for 5 min. The mixture was heated up to 30 ^{o}C and kept stirring for 1 h. Then the temperature of the reaction mixture was further increased up to 60-70 ^{o}C and stirred for another 1 h. Then it was cooled down to room temperature and poured into ice water with stirring. The greenish solid was filtered off under vacuum and washed with water and EtOH to neutral pH and dried to give compound **2** as a greenish solid in 44% yield (3.23 g, 7.80 mmol). ^{1}H NMR (300 MHz, DMSO-d_6), δ ppm: 11.22-11.17 (s, 2H), 8.38-8.34 (d, J=0.85Hz, 2H), 8.17-8.14 (s, 2H) 7.46-7.44 (d, J=1.65Hz, 2H), 7.43-7.40 (s, 2H). ^{13}C NMR (75.47 MHz, DMSO-d_6), δ ppm: 138.08, 133.76, 127.02, 126.02, 122.61, 120.85, 120.44, 110.44, 107.84, 99.22.

Synthesis of Compound 3:

To a solution of compound **2** (3 g, 7.24 mmol) in anhydrous THF (60 mL) in the 250 mL round-bottomed flask, NaH (0.905 g, 21.72 mmol) was added portion wise under a nitrogen atmosphere at 0 ^{o}C temperature, then the reaction mixture was stirred at 55 ^{o}C for 6 hrs. The reaction mixture was cooled to 0 ^{o}C again, and 2-ethyl hexyl bromide (4.20 mL, 21.72 mmol) was added drop wise to the reaction mixture. The mixture was heated to 65 ^{o}C for 36 hrs; afterwards, the solvent was removed. The residue was diluted with CH_2Cl_2 and the organic layer was washed with brine water and collected. The combined organic phase was evaporated in vacuum and purified with column chromatography on silica gel affording desired product compound **3** as yellow solid in 61% yield (2.8 g, 4.38 mmol). ^{1}H NMR (400 MHz, $CDCl_3$), δ ppm: 8.29-8.25 (d, J=1.72Hz, 2H), 7.89-7.86 (s, 2H), 7.56-7.54 (d, J=1.84Hz, 1H) 7.54-7.52 (d, J=1.72Hz, 1H), 7.26-7.25 (s, 1H), 7.25-7.23 (s, 1H), 4.22-4.19 (d,J=1.47Hz, 2H), 4.19-4.17 (d,J=2.20Hz, 2H), 2.18-2.08 (m, 2H), 1.44-1.26 (m, 16H), 0.96-0.91 (t,J=7.34Hz, 6H), 0.90-0.85 (t,J=7.09Hz, 6H). ^{13}C NMR (125.77 MHz, $CDCl_3$), δ ppm: 140.75, 136.68, 128.34, 124.29, 122.78, 122.07, 110.56, 110.06, 99.11, 47.78, 39.17, 31.00, 29.68, 28.76, 24.44, 23.05, 14.03, 10.95. FT-IR (KBr) (cm^{-1}): 3394, 2924, 1613, 1519, 1463, 1323,

1285, 1235, 1177, 1129, 1055, 1023, 880, 848, 809, 733, 669, 625, 574, 441. MS (MALDI-TOF-MS): m/z calcd for $C_{34}H_{42}Br_2N_2$, 638.17; $[M]^+$, found 638.13.

Synthesis of Compound 4:

In a mixture of compound 3 (1.7 g 2.67 mmol), Bispinacolatodiborane (2.02 g 7.98 mmol), and KOAc (0.052 g 0.53 mmol) was added 1,4-Dioxane (50 ml) and degassed for 30 minutes before addition of $[Pd(dppf)Cl_2]$ (10 mg) and subsequent degassing for 20 minutes. Then the reaction mixture was heated under nitrogen atmosphere at 80 ^oC for 24 hrs. After cooling to room temperature, the mixture was extracted with CH_2Cl_2 and the organic phase was dried over anhydrous sodium sulphate. After removal of the solvent, the residue was purified by silica gel column chromatography to get compound **4** as yellow brown solid in 68% yield (1.32 g, 1.80 mmol). ^1H NMR (400 MHz, $CDCl_3$), δ ppm: 8.69-8.67 (d, J=0.74Hz, 2H), 8.07-8.06 (s, 2H), 7.94-7.93 (d, J=1.10Hz, 1H) 7.92-7.91 (d, J=1.10Hz, 1H), 7.40-7.39 (s, 1H), 7.38-7.37 (s, 1H), 4.29-4.27 (d, J=3.43Hz, 2H), 4.27-4.25 (d, J=4.04Hz, 2H), 2.25-2.16 (m, 2H), 1.46-1.30 (m, 40H), 0.96-0.90 (t, J=7.34Hz, 6H), 0.90-0.85 (t, J=7.21Hz, 6H). ^{13}C NMR (100.62 MHz, $CDCl_3$), δ ppm: 144.23, 136.68, 132.12, 127.36, 122.82, 122.55, 108.08, 99.45, 83.52, 47.90, 39.01, 30.91, 29.68, 28.71, 24.94, 24.33, 23.12, 14.06, 10.89. FT-IR (KBr) (cm^{-1}): 2977, 2928, 1609, 1468, 1373, 1349,1288, 1177, 1127, 959, 850, 743, 710, 663, 547, 471. MS (MALDI-TOF-MS): m/z calcd for $C_{46}H_{66}B_2N_2O_4$, 732.52; $[M]^+$, found 732.58.

Synthesis of Compound 5:

In a 50 ml of two neck round bottom flask a mixture of compound **4** (1 g, 1.37 mmol), Br-BT-CHO (0.830 g, 3.42 mmol) and K_2CO_3 (2M Solution 5 mL), in THF (30 mL) solvent was degassed for 30 minutes before addition of $[Pd(PPh_3)_4]$ (5 mg) and subsequent degassing for 20 minutes. The reaction was heated under argon at 80 ^oC for 48 hrs. After cooling to room temperature, the reaction was quenched with water and extracted with CH_2Cl_2. The crude product was purified by flash column chromatography on silica gel to obtain compound **5** as red solid in 67% yield (0.728 g, 0.904 mmol). ^1H NMR (300 MHz, $CDCl_3$), δ ppm: 10.82-10.79 (s, 2H), 8.93-8.90 (d, J=0.83Hz, 2H), 8.39-8.35 (d, J=7.42Hz, 2H) 8.24-8.22 (d, J=1.37Hz, 1H), 8.22-8.19 (d, J=0.825Hz, 1H), 8.16-8.13(s, 2H), 8.08-8.03 (d, J=7.42Hz, 2H), 7.63-7.60 (s, 1H), 7.60-7.57 (s, 1H), 4.41-4.37 (d, J=5.23Hz, 2H), 4.37-4.34 (d, J=6.87Hz, 2H), 2.32-2.20 (m, 2H),1.50-1.25 (m, 16H), 1.02-0.95 (t,

J=7.15Hz, 6H), 0.94-0.86 (t, J=7.15Hz, 6H). ^{13}C NMR (100.62 MHz, $CDCl_3$), δ ppm:189.02, 142.91, 141.73, 141.65, 137.74, 137.28, 135.27, 133.10, 127.67, 126.23, 125.36, 123.33, 123.16, 121.79, 109.12, 99.76, 53.39, 47.98, 39.37, 31.04, 28.87, 24.60, 23.08, 14.14, 11.04. FT-IR (KBr) (cm^{-1}): 3415, 2921, 2856, 1735, 1682, 1610, 1534, 1465, 1320, 1263, 1213, 1164, 1130, 1014, 885, 842, 798, 752, 585, 507, 416. MS (MALDI-TOF-MS): m/z calcd for $C_{48}H_{48}N_6O_2S_2$, 804.33; $[M]^+$, found 804.37.

Synthesis of Compound ICz-Rd$_2$:

In a 50 ml of two neck round bottom flask a mixture of 3-Ethyl rhodanine (0.180 g, 1.17 mmol) and compound **5** (0.300 g, 0.372 mmol) were dissolved in dry chloroform (30 mL). Piperidine (2 drops) was then added and the mixture heated at 65 ^{o}C temperature for 24 hrs. After cooling to room temperature, the reaction was quenched with water and extracted with CH_2Cl_2 and the crude product was purified by flash column chromatography on silica gel (CH_2Cl_2) affording compound **ICz-Rd$_2$** as dark red brown solid in 31% yield (0.125 g, 0.115 mmol). ^{1}H NMR (300 MHz, $CDCl_3$), δ ppm: 8.87-8.83 (d,J=1.22Hz, 2H), 8.93-8.90 (d, J=0.83Hz, 2H), 8.57-8.55 (s, 2H) 8.20-8.18 (d, J=1.37Hz, 1H), 8.18-8.15 (d, J=1.37Hz, 1H), 8.10-8.08 (s, 2H), 7.98-7.95 (d, J=7.47Hz, 2H), 7.82-7.78 (d, J=7.62Hz, 2H), 7.56-7.54 (s, 1H), 7.54-7.52 (s, 1H), 4.40-4.29 (m, 4H), 4.27-4.24 (d, J=7.17Hz, 2H), 4.24-4.21 (d, J=7.01Hz, 2H), 2.29-2.21 (m, 2H), 1.52-1.40 (m, 12H), 1.36-1.31 (t, J=7.17Hz, 6H), 1.26-1.20 (m, 4H), 1.02-0.95 (t, J=7.32Hz, 6H), 0.94-0.87 (t, J=7.17Hz, 6H). ^{13}C NMR (100.62 MHz, $CDCl_3$), δ ppm: 193.14, 167.48, 154.74, 154.00, 153.64, 142.62, 137.18, 137.09, 131.33, 127.49, 127.38, 127.22, 126.93, 124.42, 123.26, 123.07, 121.37, 108.99, 99.65, 47.93, 39.86, 39.35, 31.04, 29.67, 29.34, 28.86, 24.58, 23.08, 22.67, 14.15, 12.30, 11.98, 11.03.FT-IR (KBr) (cm^{-1}): 3413, 2921, 2856, 1710, 1601, 1506, 1465, 1321, 1237, 1126, 891, 803, 503. MS (MALDI-TOF-MS): m/z calcd for $C_{58}H_{58}N_8O_2S_6$,1090.30; $[M]^+$, found 1090.53.

Synthesis of Compound ICz-RdCN$_2$:

In a 50 ml of two neck round bottom flask a mixture of dicyano-n-hexyl rhodanine (0.278 g, 1.116 mmol) and compound **5** (0.300 g, 0.372 mmol) were dissolved in dry chloroform (30 ml). Piperidine (2 drops) was then added and then the mixture heated at 65 ^{o}C for 24 hrs. After cooling to room temperature, the reaction was quenched with water and extracted with CH_2Cl_2 and the crude product was purified by flash column chromatography on silica gel (CH_2Cl_2) affording

compound **ICz-RdCN$_2$** as dark green solid in 28% yield (0.130 g, 4.38 mmol). ^{1}H NMR (300 MHz, $CDCl_3$), δ ppm: 8.78-8.70 (s,2H), 8.46-8.37 (s, 2H), 8.12-8.02 (d, J=7.70Hz, 2H), 7.97-7.93 (s, 2H), 7,92-7.86 (d, J=7.70Hz, 2H), 7.70-7.61 (d, J=7.21Hz, 2H), 7.48-7.39 (d, J=8.19Hz, 2H),4.45-4.29 (t, J=6.60Hz, 4H), 4.10-4.15 (d, J=7.91Hz, 2H), 4.05-4.00(d, J=7.82Hz, 2H), 2.31-2.14 (m, 2H), 1.56-1.48 (m, 8H), 1.39-1.23 (m, 24H), 1.06-0.99 (t, J=6.11Hz, 6H), 0.98-0.91 (t, J=6.48Hz, 6H), 0.90-0.84 (t, J=5.86Hz, 6H). ^{13}C NMR (100.62 MHz, $CDCl_3$), δ ppm: 166.23, 165.69, 154.37, 153.38, 142.59, 137.98, 137.25, 132.20, 130.79, 127.48, 126.67, 126.24, 123.12, 123.02, 122.94, 121.23, 117.43, 114.04, 113.24, 112.07, 108.93, 99.62, 55.64, 47.93, 45.18, 39.40, 31.90, 31.90, 31.15, 29.67, 28.91, 28.69, 25.25, 24.67, 23.11, 22.39, 14.22, 13.91, 11.07. FT-IR (KBr) (cm^{-1}): 3417, 2924, 2856, 2209, 1720, 1590, 1533, 1466, 1356, 1325, 1270, 1205, 1163, 1129, 1100, 1023, 894, 800, 726, 633, 590, 556, 517, 478. MS (MALDI-TOF-MS): m/z calcd for $C_{58}H_{58}N_8O_2S_6$, 1266.49; $[M]^+$, found 1266.23.

Measurements and Instruments:

All intermediates and final molecules were fully characterized by Nuclear Magnetic Resonance (NMR), Matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) MASS, and Fourier Transform Infrared (FT-IR) spectroscopy (**Figure S2-S25**). ^{1}H NMR and ^{13}C NMR spectra were taken in *d*-chloroform and DMSO-d_6 on Bruker AV-400 spectrometer and AV-300 NMR spectrometer instrument using tetramethylsilane (TMS) as internal reference at 298 K. Chemical shifts are presented in δ (ppm) referenced to $CDCl_3$ residual peak at 7.26 ppm and 77.0 ppm and DMSO-$d_6$peak at 2.5 ppm and 39.51 ppm for ^{1}H NMR and ^{13}C NMR, respectively.

UV-Vis absorption spectra of acceptor molecules in solution (chloroform) and thin film (on a glass substrate) were recorded using a UV-1601 Shimadzu spectrometer. The UV-Vis absorption spectra of ICz-Rd$_2$ and ICz-RdCN$_2$in chloroform and in thin film are shown in **Figure 2.**The molar extinction coefficient (ε) was obtained from the Beer-Lambert's equation,

$$I = I_o \times 10^{-\varepsilon cl} \qquad \text{(S1)}$$

Where, I and I_o are the incident and transmitted light intensity, respectively, l is the path length, and c is the analyte concentration. The calculated vs. profile is plotted in **Figure S1 (a)**. To procure thin film absorption spectra, first glass substrates were cut into pieces with size of 1 cm^2, and then vigorously cleaned in soap solution and untra-sonicated in de-ionized water and acetone sequentially for 15 min in each step and dried. To make thin film of the compounds, concentrated

solutions (15 mg·mL^{-1}) of compounds in chloroform were prepared and there after spin-coated onto clean and dry substrates at 800 rpm for 1 min.

Cyclic Voltammetry (CV) experiments were performed in deoxygenated dichloromethane solution. All measurements were carried out at room temperature with a conventional three electrode cell consisting of a platinum wire working electrode, platinum mesh counter electrode and Ag/Ag+ reference electrode was in saturated KCl, calibrated against ferrocene as standard. Tetrabutylammonium perchlorate (TBAP 0.1 M) in dichloromethane (DCM) solution was used as supporting electrolyte and the potential scan rate was 100mV.s^{-1}. A ferrocene/ferrocenium (Fc/Fc+) redox couple was used as an external standard. The HOMO energy levels of molecules were estimated from the onset of first oxidation waves in CV **Figure S1(b)**. The energy band gaps of acceptors were measured from onset of absorption spectra in solution (**Figure 2**). The LUMO energy level of molecules were calculated by using the equation,

$$E_{HOMO} = -(4.80 + E_{ox}^{onset}) \quad \text{(S2)}$$

$$E_{LUMO} = E_{HOMO} + E_{g,opt} \quad \text{(S3)}$$

While the optical band gap of molecule calculated from the onset of the absorption profile (**Fig. 3)** and the optoelectronic properties are summarized in **Table 1**.

Device Fabrication and Characterization:

The PSCs were fabricated with a conventional device architecture, i.e. ITO coated glass/PEDPOT:PSS/P:**ICz-Rd$_2$** or **ICz-RdCN$_2$**/PFN/Al. Firstly, all of the ITO coated glass substrates were cleaned by successive sonication in detergent, deionized water, acetone and finally isopropanol (10 min in each step) and then dried in a vacuum oven for 1 hour. The PEDOT:PSS solution was spin-coated onto the clean ITO substrates at 2000 rpm followed by baking at 120 °C for 15 min in air. The active layer materials (**P: ICz-Rd$_2$** or **ICz-RdCN$_2$** with different weight ratio) were dissolved in chloroform (CF) and then spin-coated onto the top of the PEDOT:PSS layer at 2500 rpm for 60 sunder inert atmosphere (weight ratio of $PC_{71}BM$ kept constant) followed by thermal annealing treatment at 40 °C for 10 min. For the solvent vapour annealing the active layers were placed in a Petri-dish containing CS_2 for 40 s and then removed. A methanol solution of PFN (1.5 mg/mL) was then spin-coated on top of the active layer at 3000 rpm for 30 s. The thickness of the active layers was 90±5 nm. Finally, an Al top electrode was deposited onto the

top of the PFN buffer layer by thermal evaporation at vacuum pressure of 2.0×10^{-5} Pa. The effective area of the devices was around 16 mm^2. OSCs based on binary BHJ active layers were also prepared for comparison. The current–voltage (J–V) characteristics of the BHJ organic solar cells were measured using a computer-controlled Keithley 2400 source meter in the dark and under a simulated AM 1.5G illumination of 100 mW/cm^2. A Xenon light source coupled with an optical filter was used to provide the stimulated irradiance at the surface of the devices. The incident photon to current efficiency (IPCE) of the devices was measured by illuminating the device through the light source and the monochromator and the resulting current was measured using a Keithley electrometer under short circuit conditions.

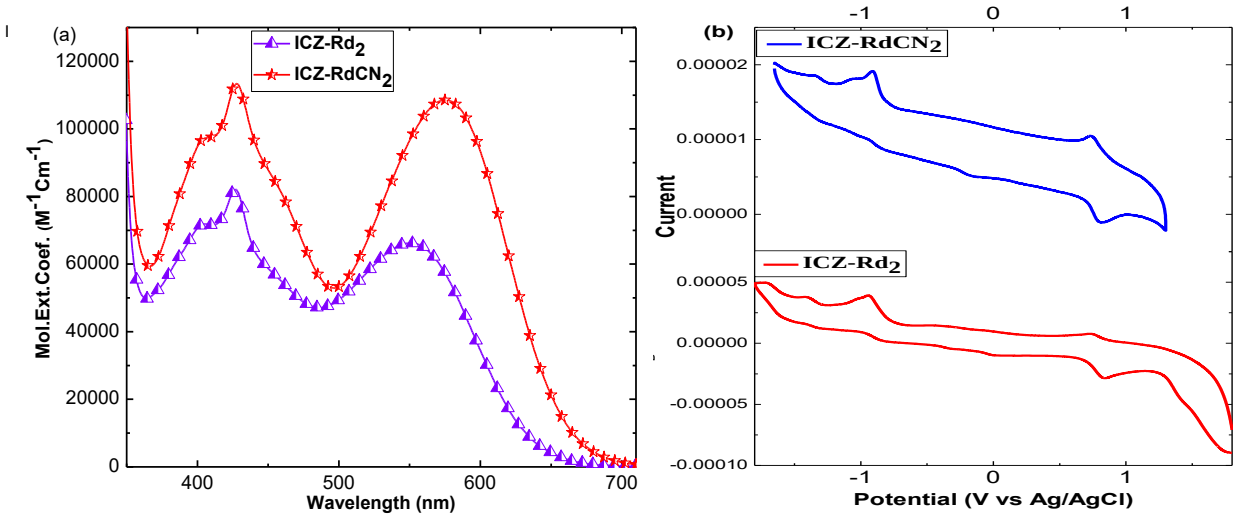


Figure S1. (a) Molar extinction coefficient and (b) Cyclic voltagram (CV) of **ICz-Rd$_2$** and **ICz-RdCN$_2$**.

Table S1 Optoelectronic properties of**ICz-Rd$_2$** and **ICz-RdCN$_2$:**

Molecules	HOMO[a] (eV)	LUMO[a] (eV)	E^a_g (eV)	λ^a_{max} (nm) (solution)	ε^a ($M^{-1}.cm^{-1}$)	HOMO[b] (eV)	LUMO[b] (eV)	E^b_g (eV)	E^b ($Mol^{-1}.cm^{-1}$)
ICz-Rd$_2$	-5.59	-3.88	1.71	543 nm	6.65×10^4	-5.17	-3.70	1.47	1.42×10^5
ICz-RdCN$_2$	-5.58	-3.98	1.61	582 nm	1.08×10^5	-5.52	-4.14	1.38	2.78×10^5

[a] Experimental data, [b]calculated data at DFT/CAM-B3LYP/6-311g(d,p)

Table S2 Major allowed transition in the range of 280-600 nm of **ICz-Rd$_2$** and **ICz-RdCN$_2$** calculated at DFT using CAM-B3LYP/6-311g (d,p) level.

Molecules	Excited state	$\lambda_{(nm)}$	Osc. Strength (*f*)	Major transitions
ICz-Rd$_2$	S1	494	2.55	H-2→L+1 (32%), HOMO→LUMO (53%)
	S2	477	0.01	H-2→LUMO (35%), HOMO→L+1 (51%),
	S3	361	0.14	H-3→LUMO (11%), H-1→LUMO (41%), HOMO→L+4 (29%)
	S4	352	0.0	H-3→L+1 (15%), H-1→L+1 (57%)
	S5	303	0.70	H-1→L+4 (69%)
ICz-RdCN$_2$	S1	515	1.55	HOMO→L+1 (75%)
	S2	495	0.46	H-4→L+2 (12%), H-1→LUMO (51%)
	S3	389	0.02	H-1→LUMO (10%), HOMO→LUMO (75%)
	S4	320	0.03	HOMO→L+5 (68%)
	S5	319	0.07	HOMO→L+2 (76%)

Table S3 Photovoltaic performance of carbazole based NFAs:

Acceptors	Eg (eV)	LUMO (eV)	Donor	Jsc (mA cm^{-2})	Voc (V)	FF (%)	PCE (%)	Ref.
Cz-RH	2.03	-3.50	P3HT	4.69	1.03	53	2.56	[3]
Cz-IN	1.99	-3.37	P3HT	0.13	0.61	26	0.02 (0.02)	[4]
Cz-ECA	2.15	-3.37	P3HT	2.34	1.00	44	1.03 (0.98)	[4]
CBM	2.02	-3.64	PCE10	10.6	0.88	53	5.3 (5.0)	[5]
N7	1.82	-3.74	P3HT	3.16	1.17	62	2.3	[6]
DTCC-IC	1.59	-3.87	PTB7-Th	11.23	0.95	56.2	6 (5.74)	[7]
DTPC-IC	1.24	-3.97	PTB7-Th	8.53	0.863	42.4	3.12 (2.86)	[8]
DTPC-DFIC	1.21	-4.10	PTB7-Th	21.92	0.760	61.3	10.21 (10.01)	[8]
ICz-Rd$_2$	1.83	-3.76	P	14.04	1.04	54	7.88	This work
ICz-RdCN$_2$	1.76	-3.82	P	15.58	1.01	62	9.76	This work

NMR, MALDI-TOF and FT-IR spectra

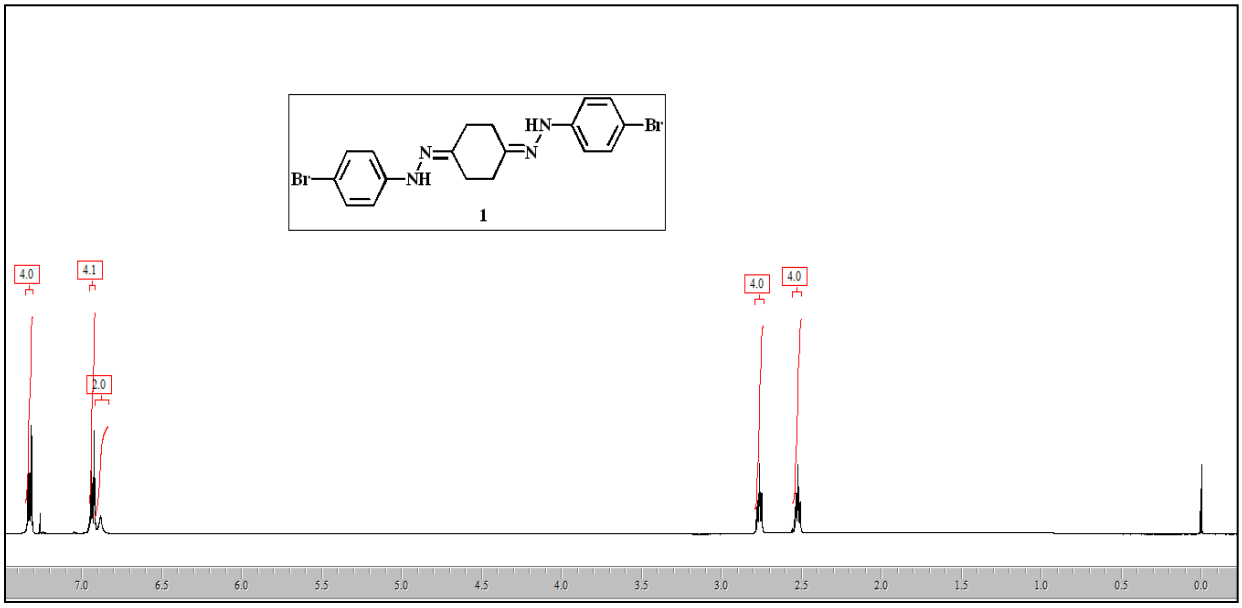


Figure S2. ^{1}H NMR of compound 1 in $CDCl_3$.

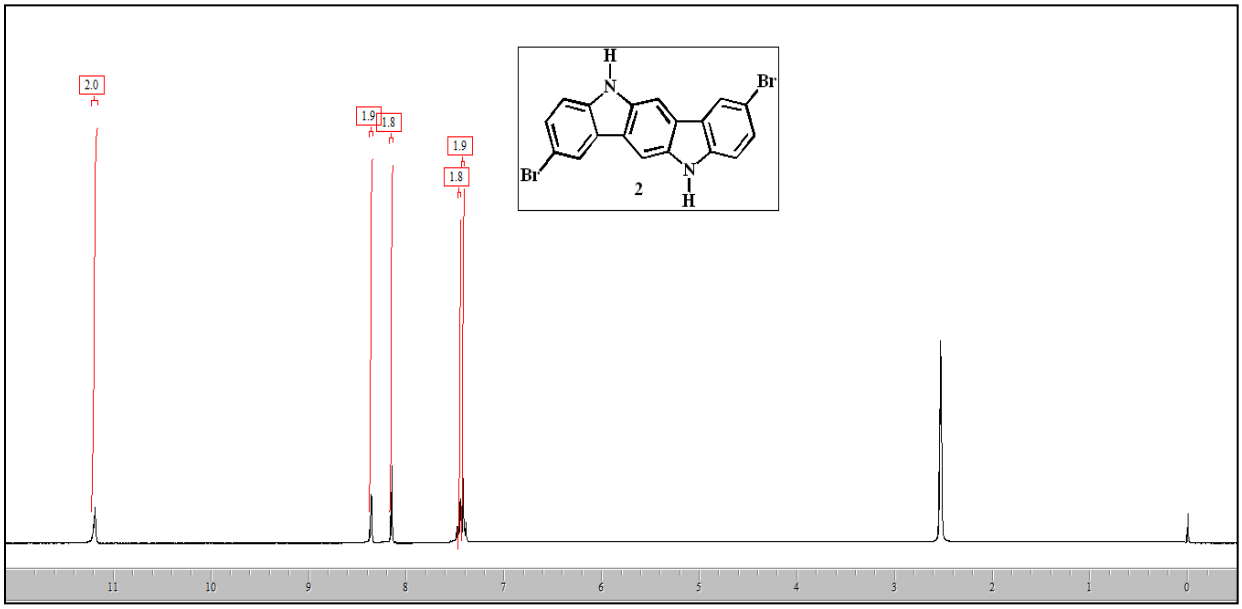


Figure S3. ^{1}H NMR of compound 2 in DMSO-d_6.

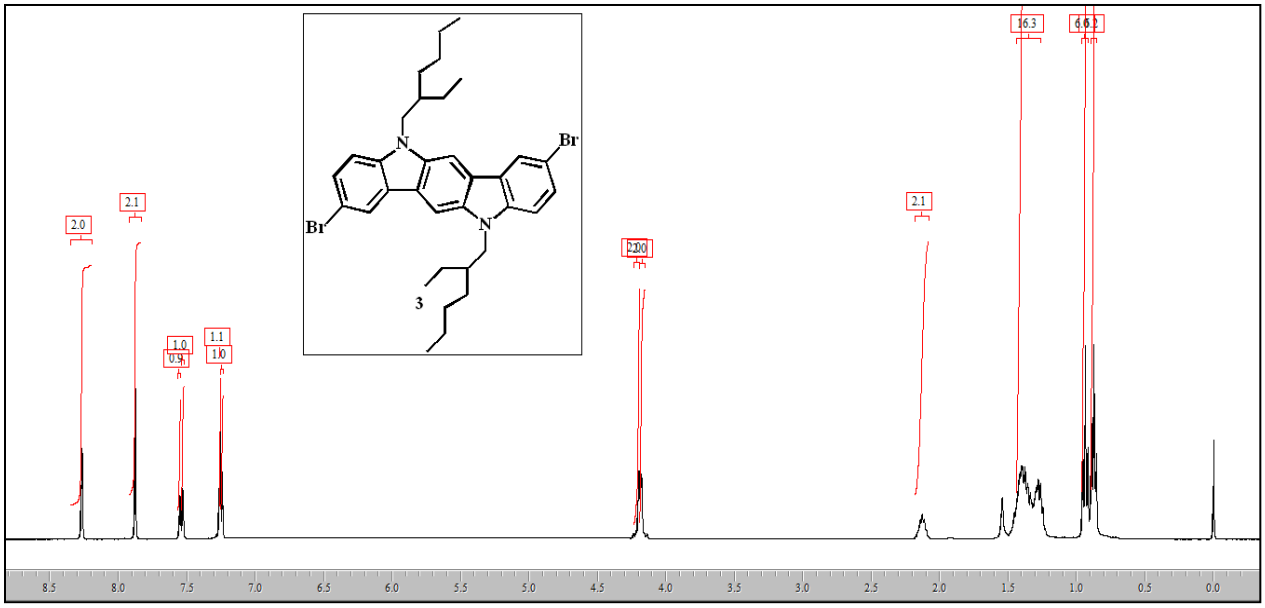


Figure S4. ^{1}H NMR of compound 3 in $CDCl_3$.

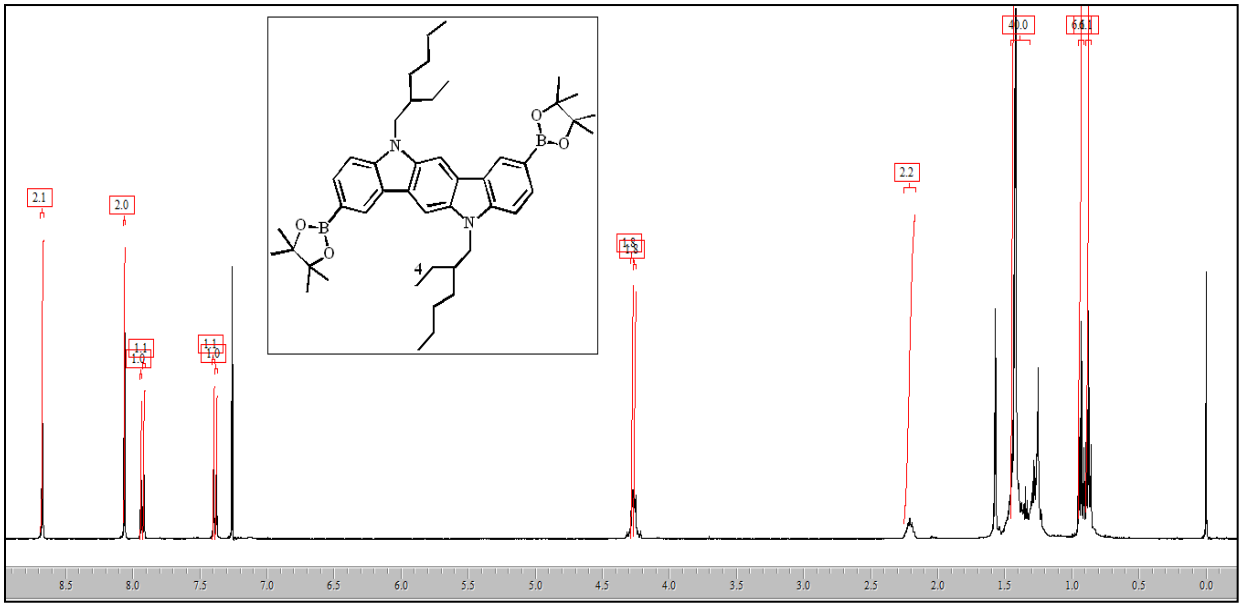


Figure S5. ^{1}H NMR of compound 4 in $CDCl_3$.

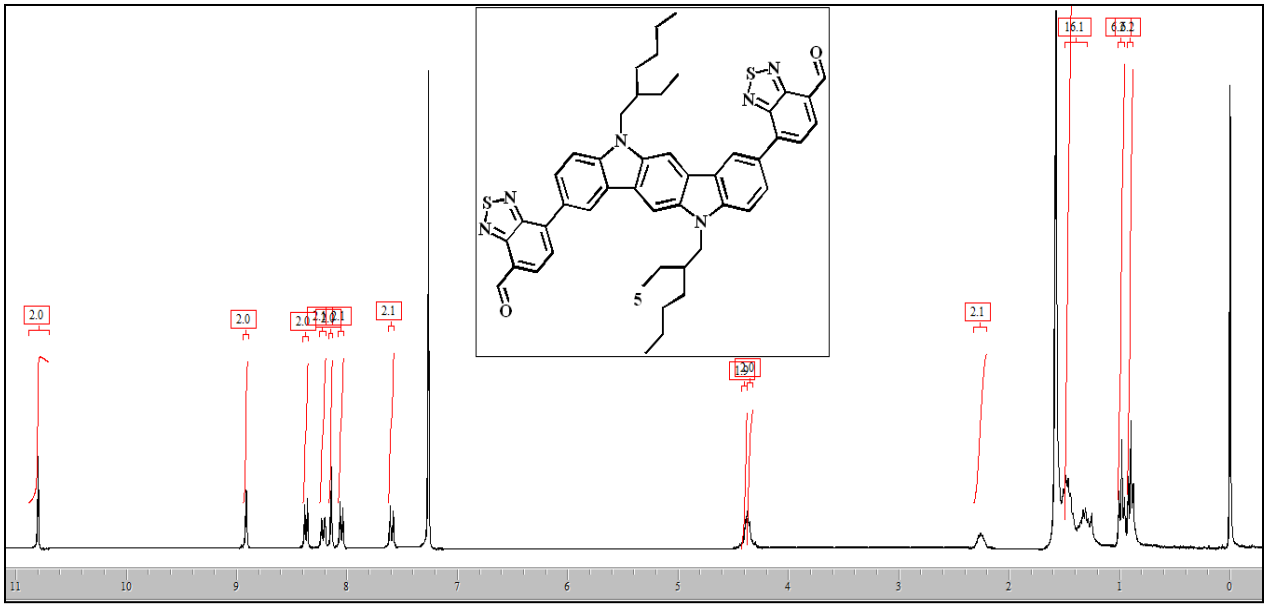


Figure S6. ^{1}H NMR of compound 5 in $CDCl_3$.

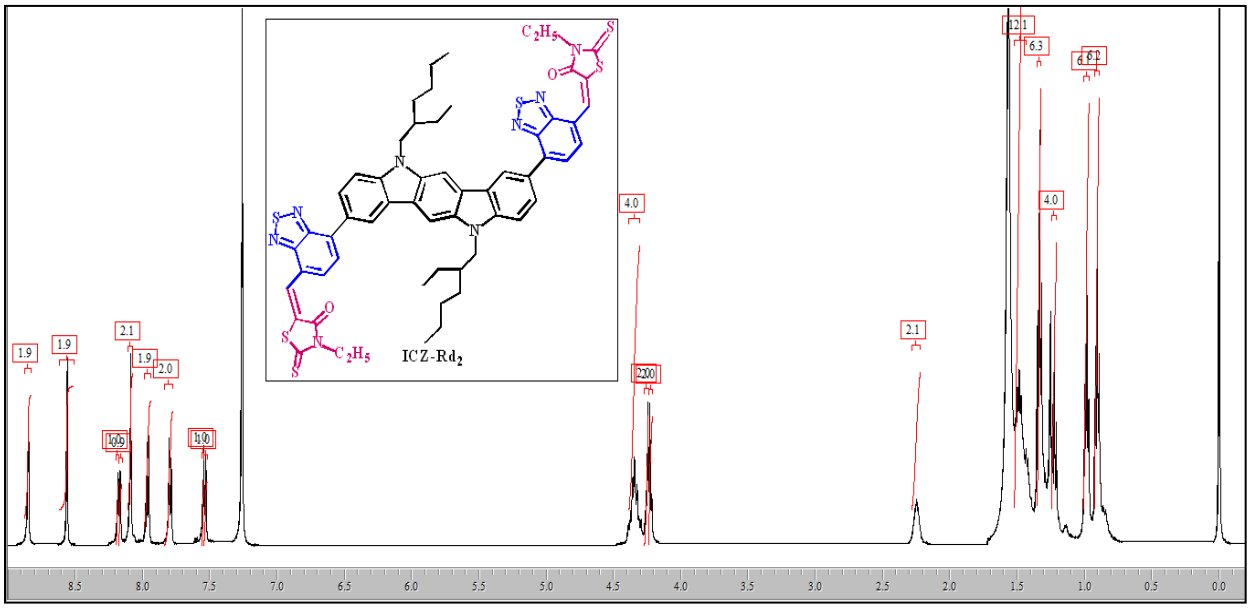


Figure S7. ^{1}H NMR of **ICz-Rd2** in $CDCl_3$.

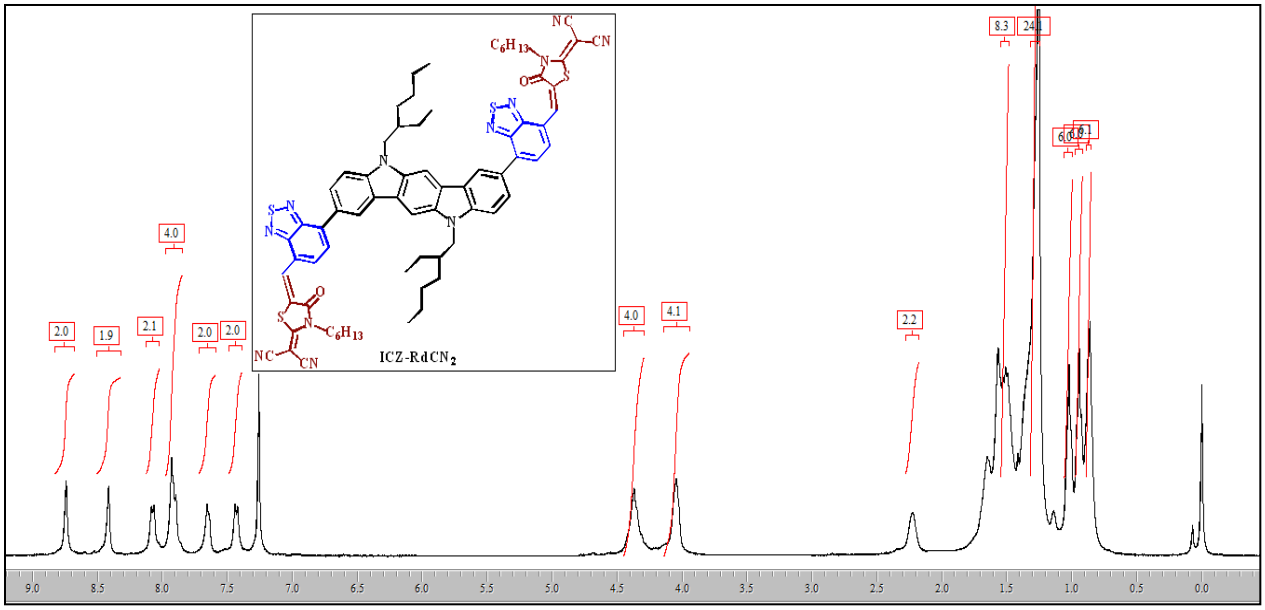


Figure S8. ^{1}H NMR of **ICz-RdCN$_2$** in $CDCl_3$.

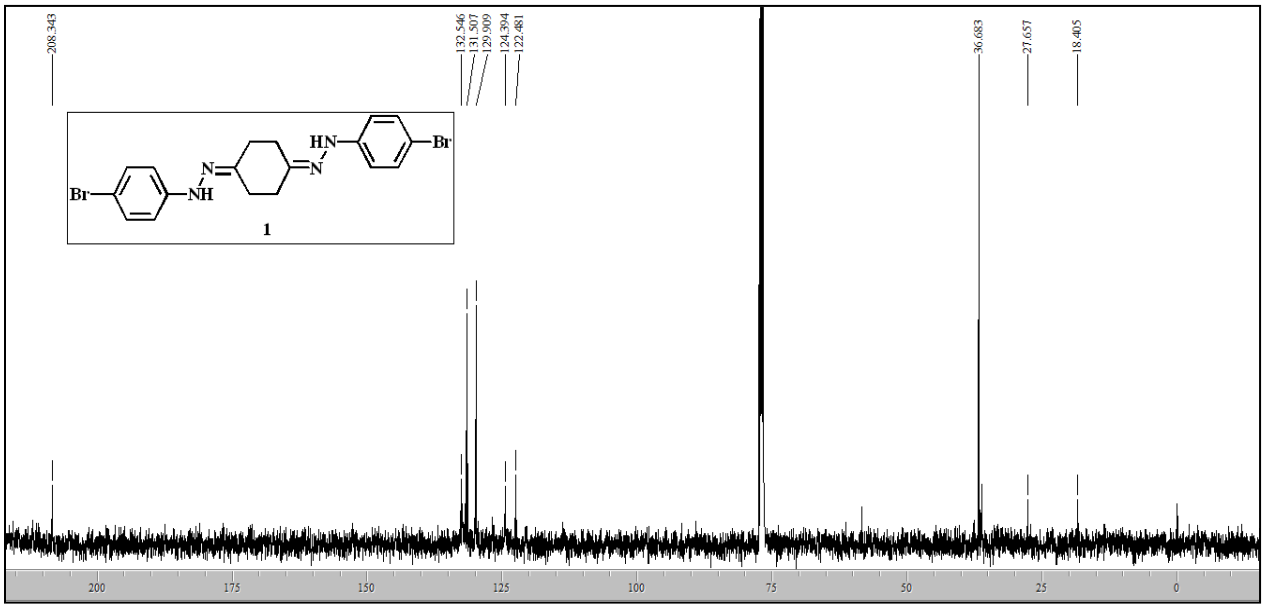


Figure S9. ^{13}C NMR of compound 1 in $CDCl_3$.

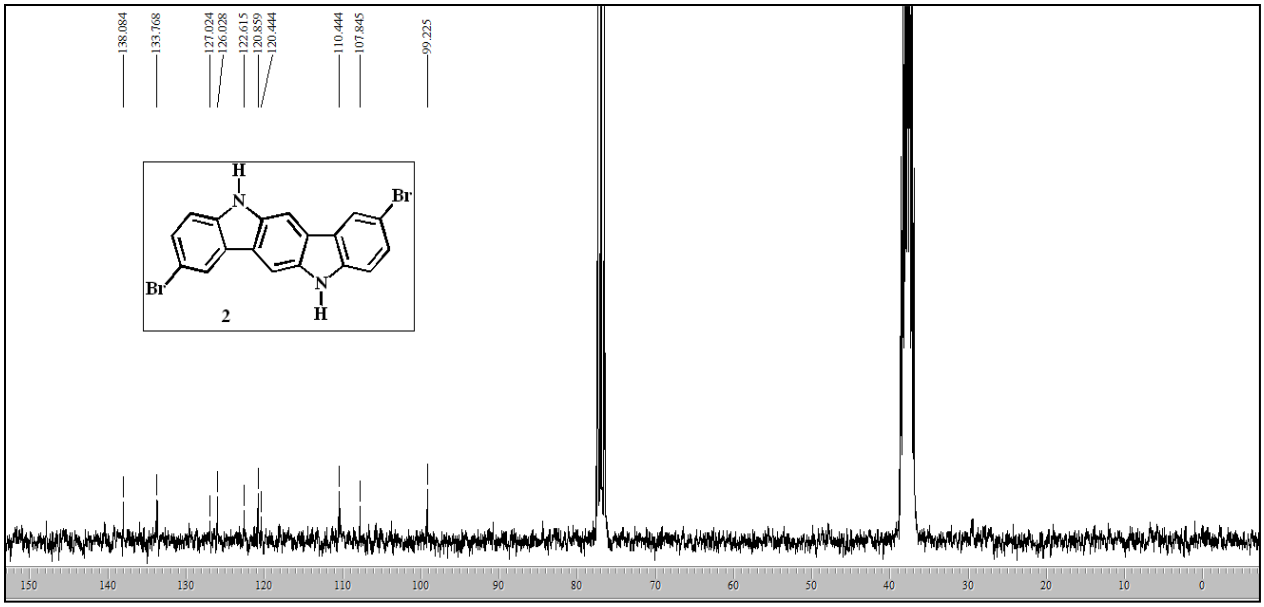


Figure S10. ^{13}C NMR of compound 2 in DMSO-d_6.

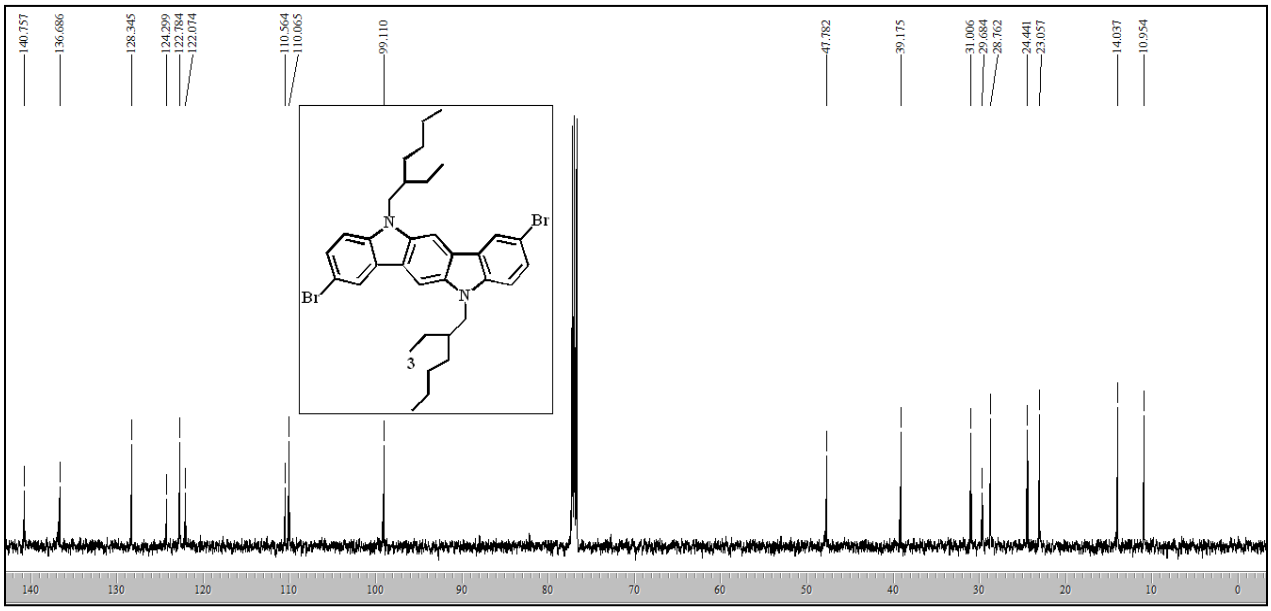


Figure S11. ^{13}C NMR of compound 3 in $CDCl_3$.

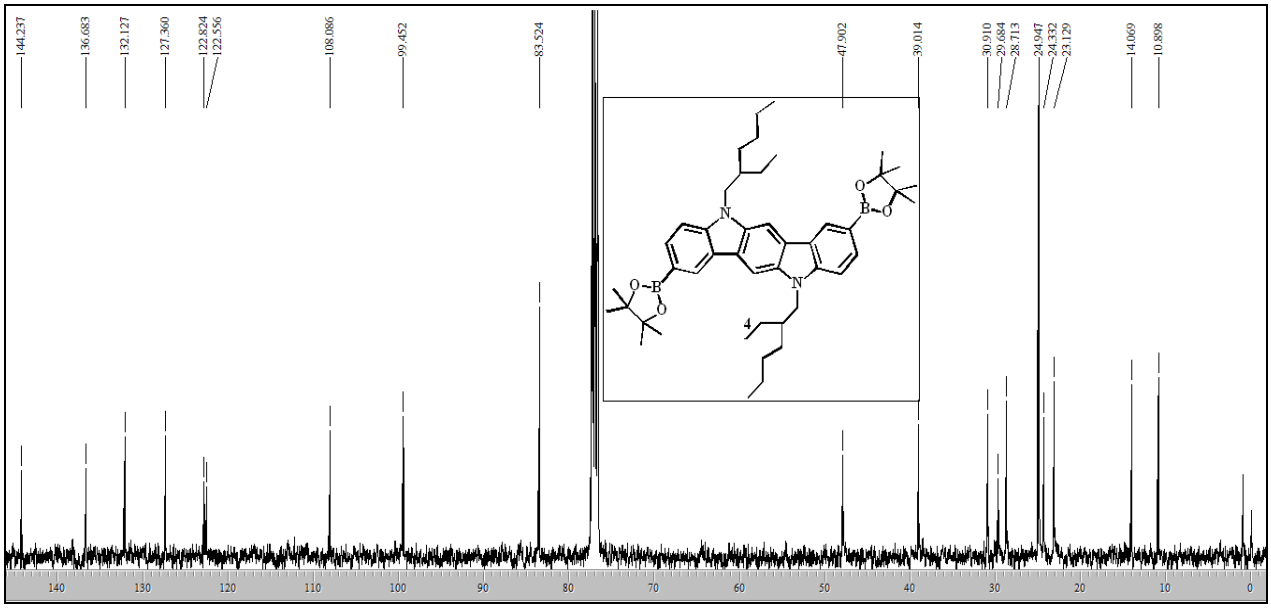


Figure S12. ^{13}C NMR of compound 4 in $CDCl_3$.

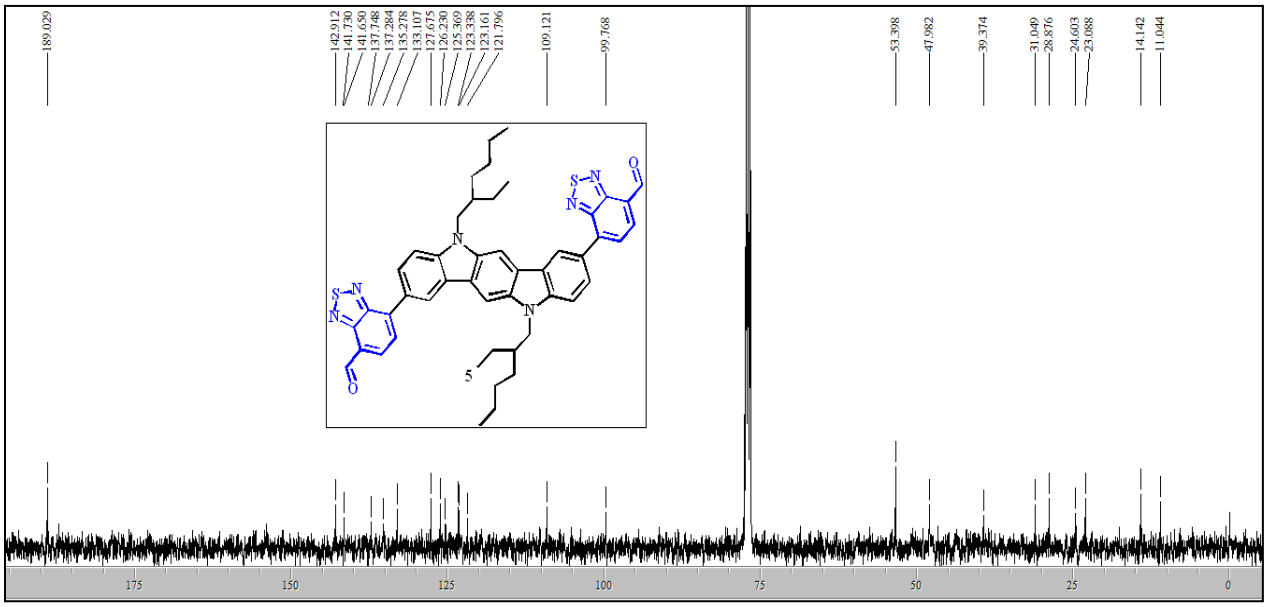


Figure S13. ^{13}C NMR of compound 5 in $CDCl_3$.

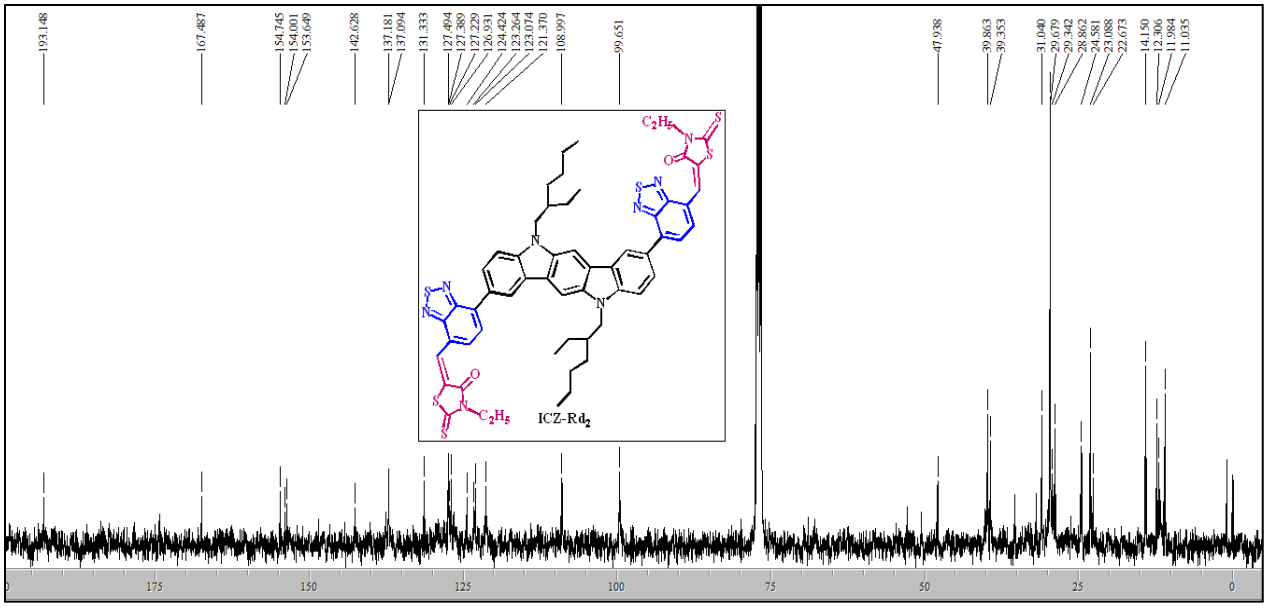


Figure S14. ^{13}C NMR of **ICz-Rd2** in $CDCl_3$.

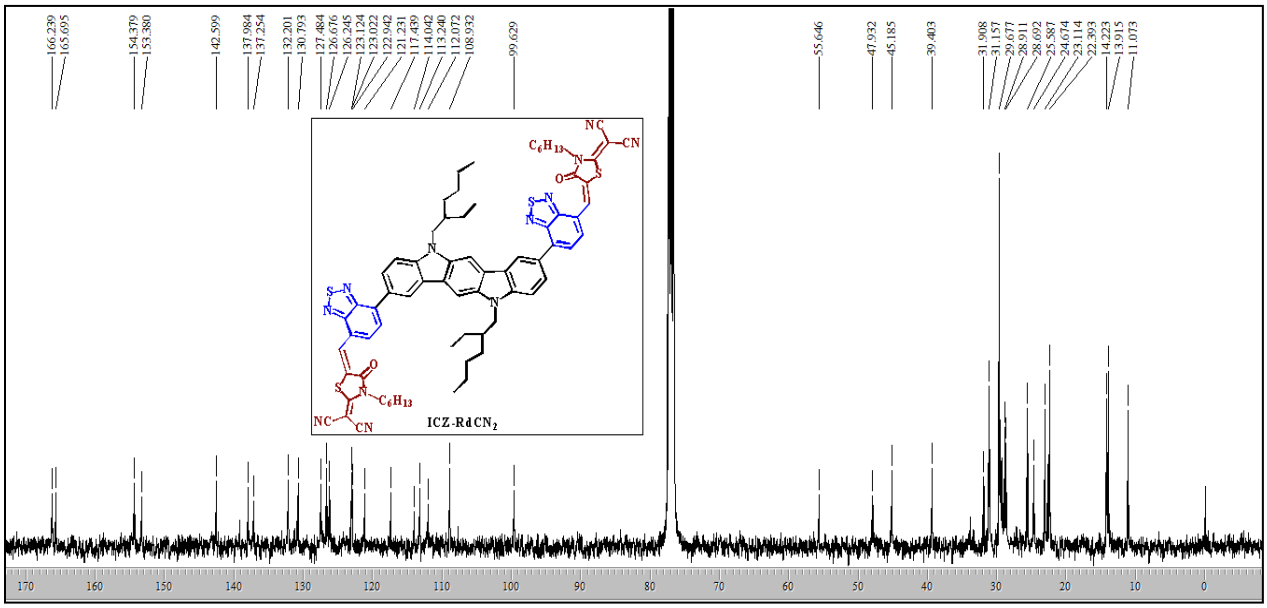


Figure S15. ^{13}C NMR of **ICz-RdCN2** in $CDCl_3$.

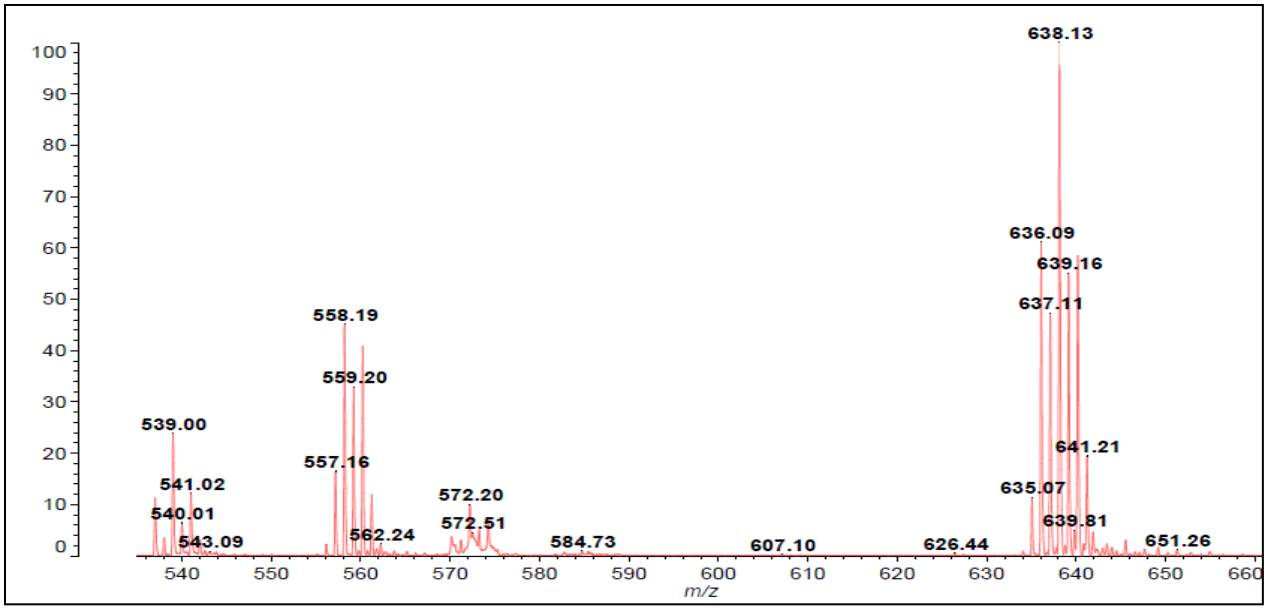


Figure S16. MALDI-TOF spectra of compound 3**.**

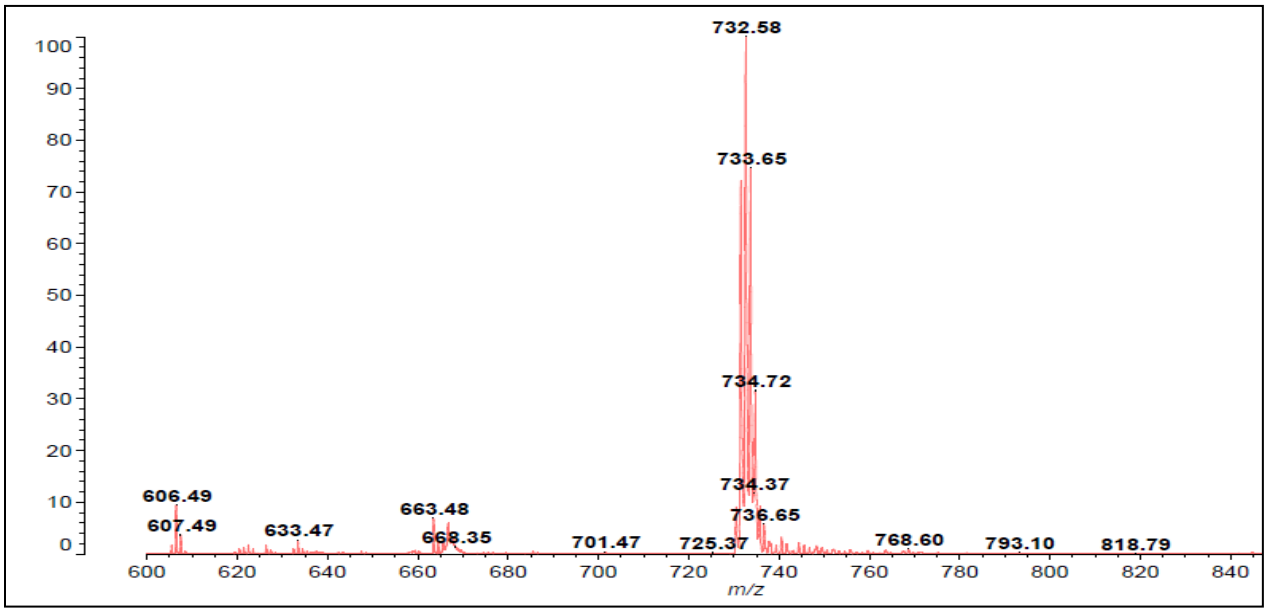


Figure S17. MALDI-TOF spectra of compound 4**.**

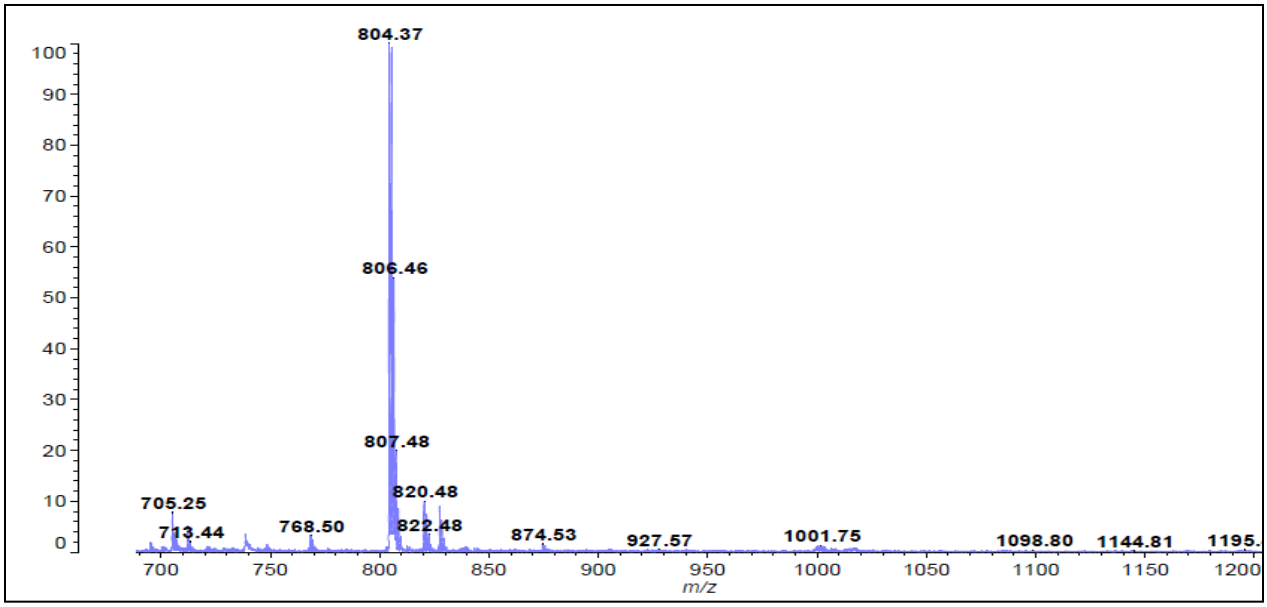


Figure S18. MALDI-TOF spectra of compound 5**.**

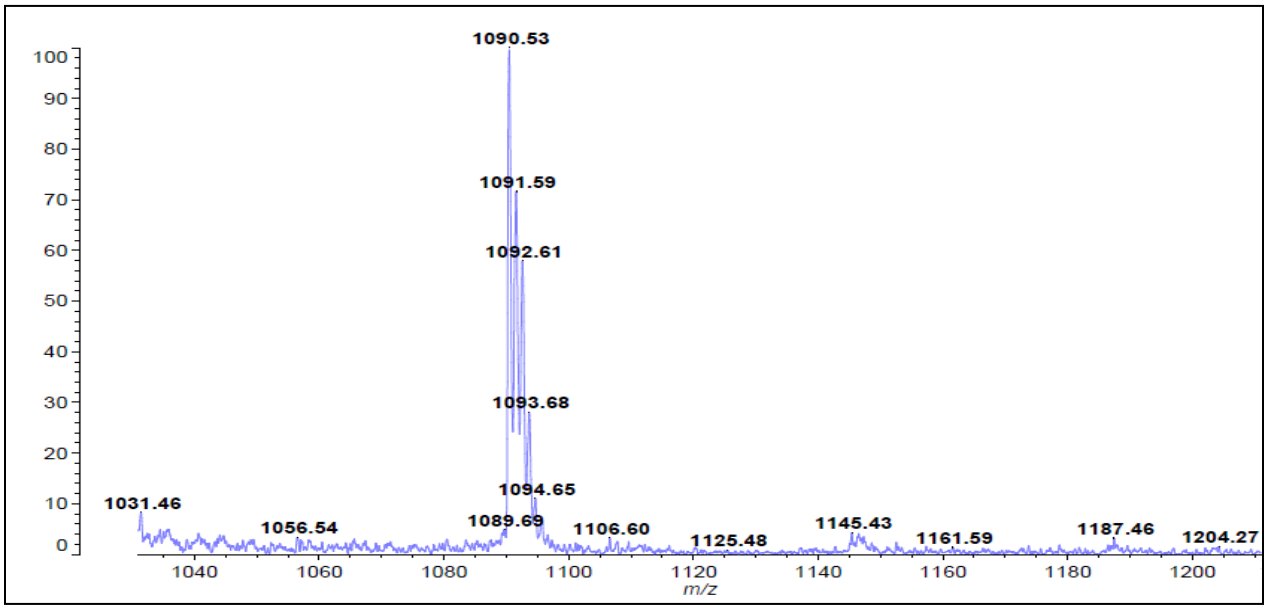


Figure S19. MALDI-TOF spectra of compound **ICz-Rd$_2$.**

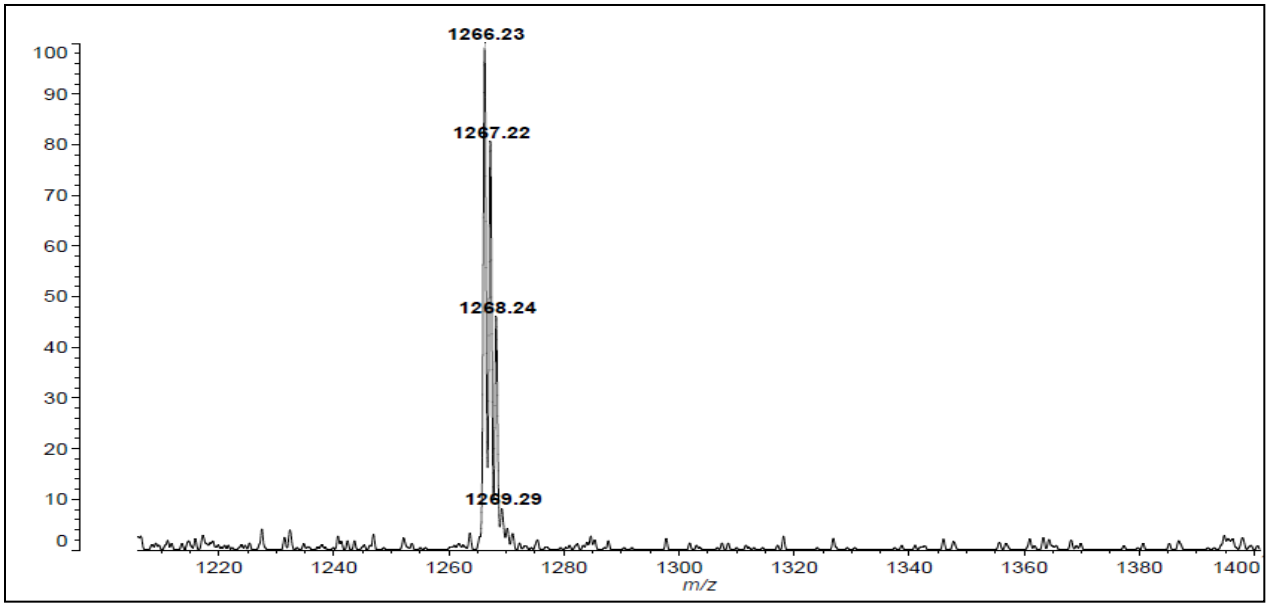


Figure S20. MALDI-TOF spectra of compound **ICz-RdCN2.**

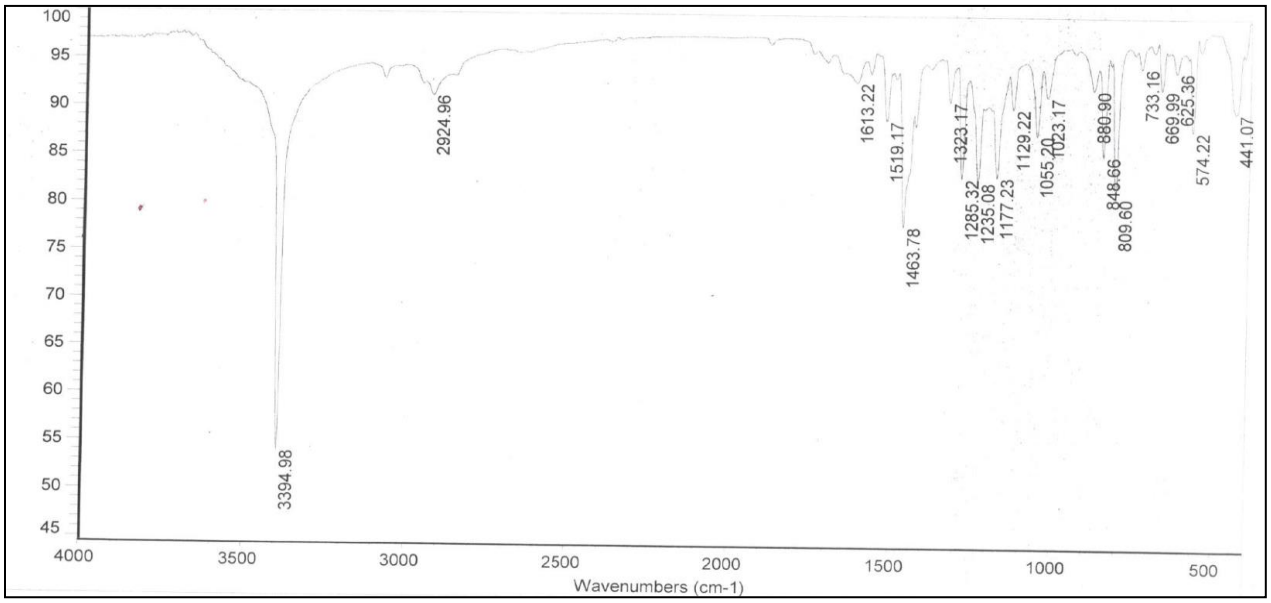


Figure S21. FT-IR spectra of compound 3.

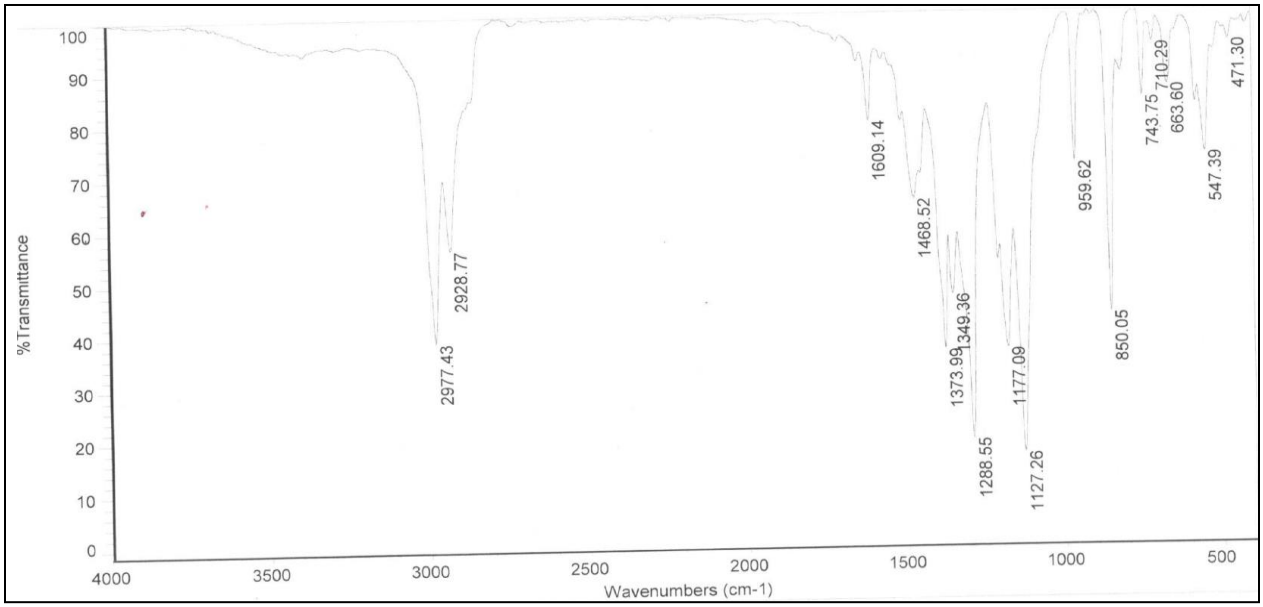


Figure S22. FT-IR spectra of compound 4.

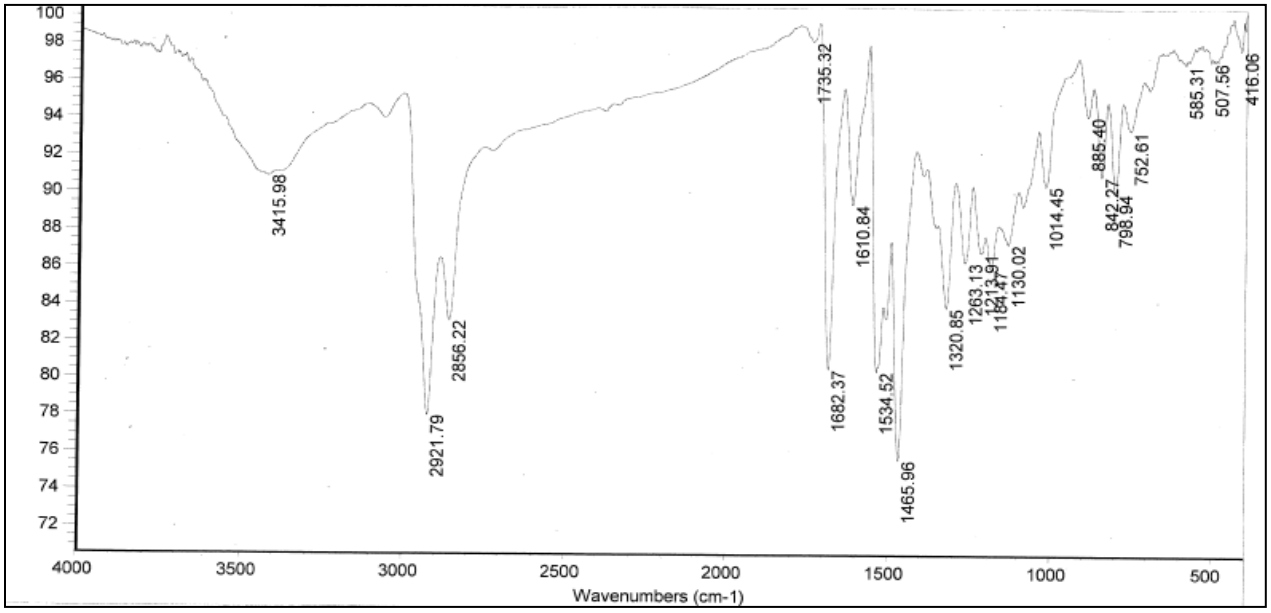


Figure S23. FT-IR spectra of compound 5.

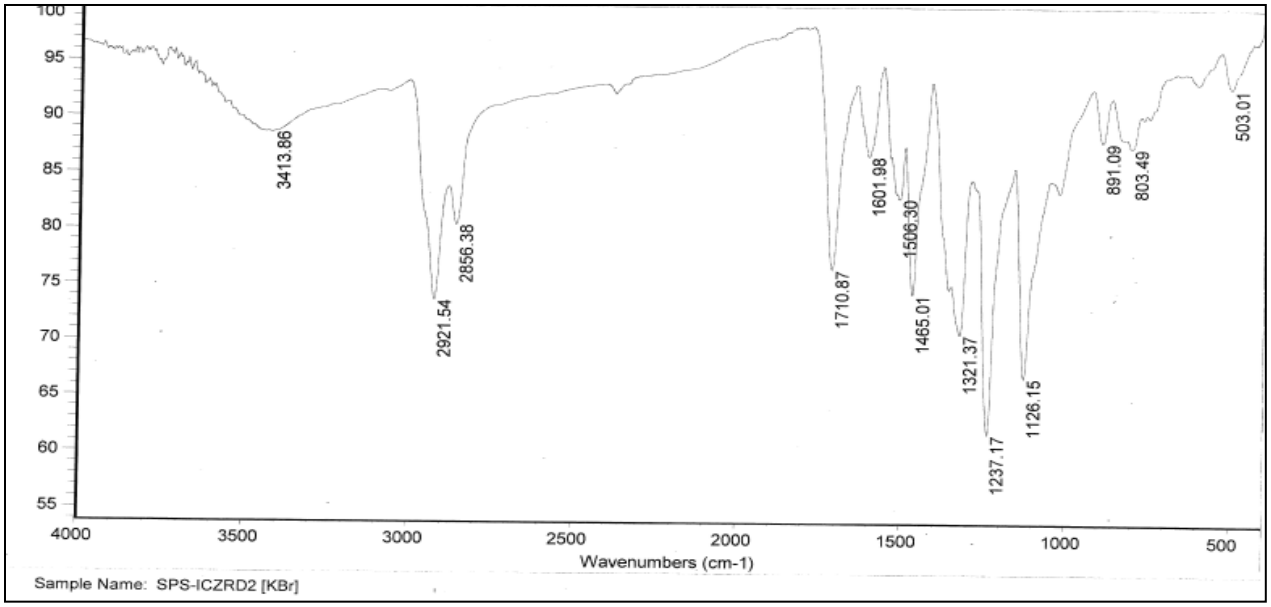


Figure S24. FT-IR spectra of **ICz-Rd$_2$.**

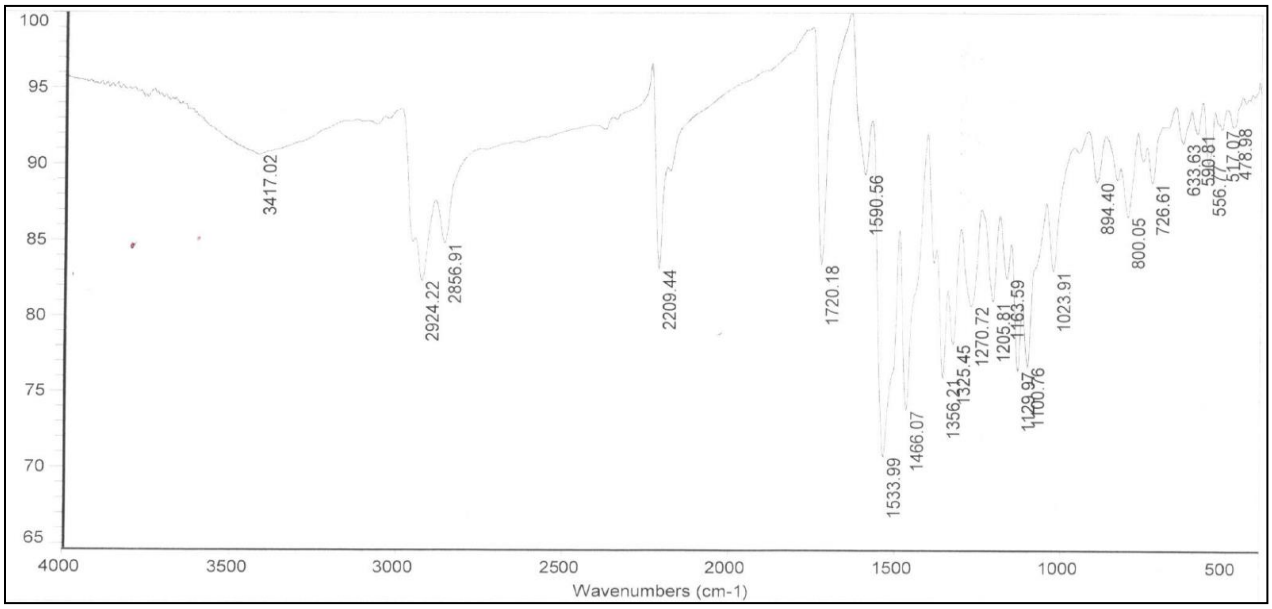


Figure S25. FT-IR spectra of **ICz-RdCN$_2$.**

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