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Contorted Graphene Nanoribbons From Vat Dyes: Synthesis, Properties and Charge Carrier Mobility

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Apparatus

Nuclear Magnetic Resonance (NMR) spectra were acquired using a Varian Inova AS400 spectrometer (Varian, Palo Alto, USA) operating at 400 MHz or an Agilent DD2 500 MHz spectrometer. Signal notations include s (singlet), d (doublet), t (triplet), dd (doublet of doublets), dt (doublet of triplets), m (multiplet), and coupling constants (*J*) expressed in hertz (Hz). Chemical shifts are presented in parts per million (ppm) relative to the residual solvent peak.

High-resolution mass spectra (HRMS) were obtained using an Agilent 6210 time-of-flight (TOF) LCMS apparatus equipped with an ESI and APPI ion source (Agilent Technologies, Toronto, Canada). Number-average (M_n) and weight-average (M_w) molecular weights were determined through size-exclusion chromatography (SEC) using a high-temperature GPC-TOSOH EcoSEC HT. The column set comprised 2 PL gel Mixed C (300 x 7.5 mm) columns and a PL gel Mixed C guard column. The eluent used was 1,2,4-trichlorobenzene (TCB) (with 0.0125% BHT w/v) at a fixed flow rate of 1 $mL\cdot min^{-1}$, and the system temperature was set at 110 ºC. Samples were prepared at a nominal concentration of 1.0 $mg\cdot mL^{-1}$ in 1,2,4-trichlorobenzene (TCB). Dissolution was conducted using a Varian Polymer Laboratories PL-SP 260VC sample preparation system, with sample vials held at 110 ºC and shaken for 1 hour for complete dissolution. The resulting solutions were filtered through a 2 mm porous stainless-steel filter combined with a 0.40 mm glass filter into a 4 mL chromatography vial. The calibration method employed was the classical polystyrene method, utilizing polystyrene narrow standards (Easi-Vials PS-M from Varian Polymer Laboratories) dissolved in (TCB).

UV-visible spectra of monomers were recorded on a Varian diode-array spectrophotometer (model Cary 7000) using 10 mm path length quartz cells. Cyclic voltammograms (CVs) were measured on a Solartron 1287 potentiostat with platinum electrodes at a scan rate of 50 $mV\cdot s^{-1}$. An Ag/Ag^+ (0.01 M $AgNO_3$ in acetonitrile) reference electrode was used in an anhydrous and argon-saturated solution of 0.1 M tetrabutylammonium tetrafluoroborate (Bu_4NBF_4) in acetonitrile. Tetrabutylammonium tetrafluoroborate (98%, Aldrich) was recrystallized from methanol/water and dried at 70 °C under reduced pressure. Under these conditions, for a freshly prepared reference electrode, the half-wave oxidation potential (E½) of ferrocene should be approximately 0.091 V versus Ag/Ag$^+$, as reported by Li *et al*. The Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energy levels are determined from the onset of oxidation and reduction, respectively. The onset potentials are determined at the position where the current starts to deviate from the baseline.

$$E_{HOMO} = -\left[\left(E'_{ox\ vs\ Ag/Ag^+}\right) - \left(E^{1/2}_{Ferrocene\ vs\ Ag/Ag^+}\right) + 4.8\right]$$

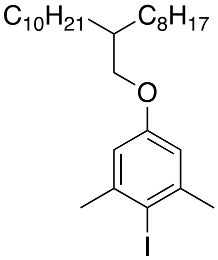
General Methods

Chemical reagents were purchased from Sigma–Aldrich Co. Canada, Oakwood Products, Inc. or Strem Chemicals, Inc. and were used as received. Vat Orange 1 was purchased from Hangzhou Chungyo Chemical Co. Ltd.

OFET device

Bottom-gate top-contact (BGTC) OFET devices were fabricated on a highly doped *n*-type Si(100) wafer with a 300 nm-thick SiO_2 dielectric layer. Wafers were first functionalized with an n-octadecyltrimethoxysilane (OTS) self-assembled monolayer, according to reported methods.[1] The OTS-treated substrate was sonicated with toluene, acetone, and isopropanol, then dried with nitrogen before use. Prepared solutions of the polymer blends (5 mg/mL) were filtered and spin-coated onto the substrates at 1000rpm for 1 minute to form thin films approximately 50μm thick. Thermal annealing was carried out using a hot plate at 150 °C for 30 minutes inside a glove box under a N_2 atmosphere. Gold source and drain contacts were then deposited through a shadow mask via e-beam physical vapor deposition. 50 nm of Au (2 Å s−1) was deposited on top of the polymer films, yielding devices with channel length L and width W defined as 100 and 1000µm, respectively. Measurements of the device characteristics were conducted at room temperature using a Keithley 4200-SCS semiconductor parameter analyzer (Keithley Instruments Inc., Cleveland, OH, USA) inside a N_2-purged glovebox.

Synthesis



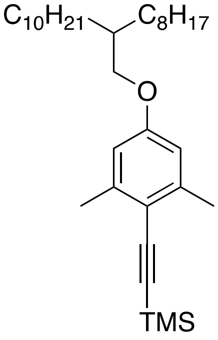
Compound 1: To a solution containing 4-iodo-3,5-dimethylphenol (9.92 g, 40.0 mmol) in 120 mL of tetrahydrofuran (THF), triphenylphosphine (12.6 g, 48.0 mmol), diisopropyl azodicarboxylate (DIAD) (8.70 g, 48.0 mmol, 10 mL), and 2-octyldodecanol (14.3 g, 48.0 mmol, 12 mL) were added. The resulting mixture was stirred at room temperature for 14 hours. Dichloromethane was added and the mixture was washed with brine. The combine organic layers were dried using anhydrous sodium sulfate. The solvent was removed under vacuum and the crude product was purified by

column chromatography (silica gel, hexanes as the eluent) to provide the desired compound as a colorless liquid (15.0 g, 71%).

^{1}H NMR (500 MHz, CDCl$_3$) δ = 6.69 – 6.65 (m, 2H), 3.79 (d, *J* = 5.6 Hz, 2H), 2.44 (s, 6H), 1.75 (t, *J* = 6.1 Hz, 1H), 1.47 – 1.23 (m, 38H), 0.94 – 0.85 (m, 6H).

^{13}C NMR (126 MHz, CDCl$_3$) δ = 159.0, 142.7, 113.5, 96.6, 70.8, 38.0, 34.5, 32.0 (2x), 31.4, 30.1, 29.7 (4x), 29.4 (2x), 26.9, 22.8, 22.7, 14.2.

HRMS (ESI$^+$): m/z calcd for $C_{28}H_{49}OI$: 528.2823; found: 528.2815 [M]$^+$, diff = 1.42 ppm.

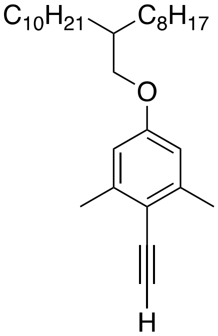


Compound 2: A degassed round bottom flask was charged with compound **1** (5.28 g, 10.0 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (115 mg, 0.10 mmol), CuI (38 mg, 0.20 mmol), toluene (40 mL) and diisopropylamine (DIPA) (10 mL). The resulting mixture was warmed to 60 °C. A solution of trimethylsilylacetylene (1.50 g, 2.17 mL, 15.0 mmol) in toluene (40 mL) and DIPA (10 mL) was added to the mixture under nitrogen flow. The resulting mixture was refluxed for 18 hours, subsequently cooled to room temperature, and then diluted with CH$_2$Cl$_2$ (50 mL). The mixture was washed with 10% aqueous NH$_4$OH, water and brine. The organic phase was washed, dried with MgSO$_4$, filtered and the solvent was removed under reduced pressure. The remaining residue was purified by column chromatography (silica gel, hexanes as the eluent) to provide compound **2** as a pale-yellow oil (3.74 g, 75%).

^{1}H NMR (500 MHz, CDCl$_3$) δ = 6.63 – 6.59 (m, 2H), 3.84 (d, *J* = 5.7 Hz, 2H), 2.45 (q, *J* = 0.7 Hz, 6H), 1.79 (t, *J* = 6.1 Hz, 1H), 1.51 – 1.25 (m, 31H), 0.93 (td, *J* = 7.0, 0.9 Hz, 6H), 0.33 – 0.25 (m, 9H).

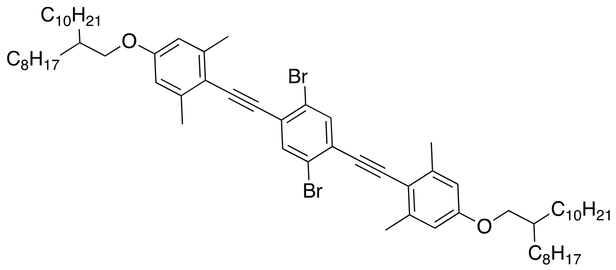
^{13}C NMR (126 MHz, $CDCl_3$) δ = 158.9, 142.3, 115.1, 112.9, 103.2, 100.6, 70.7, 38.0, 32.0 (2x), 31.4, 30.0, 29.7 (3x), 29.6, 29.4, 29.4, 26.9, 22.7 (2x), 21.3, 14.2, 0.3.

HRMS (ESI$^+$): m/z calcd for $C_{33}H_{58}OSi$: 499.4290; found: 499.4318 $[M+H]^+$, diff = 5.61 ppm.



Compound 3: A solution of compound **2** (5.00 g, 10.0 mmol) in methanol (30 mL) was treated with K_2CO_3 (13.1 g, 95.0 mmol). The reaction mixture was stirred for 18 hours at room temperature. After removing the solvent under reduced pressure, the resulting residue was filtered through a Celite pad using hexane as the eluent (80 mL). The filtrate was then evaporated under reduced pressure, and the crude product was subjected to purification via silica gel column chromatography with hexane. This purification process afforded compound 3 as a white waxy solid (3.75 g, 88%).

^{1}H NMR (500 MHz, $CDCl_3$) δ = 6.60 (s, 2H), 3.81 (d, *J* = 5.6 Hz, 2H), 3.42 (d, *J* = 1.4 Hz, 1H), 2.43 (s, 6H), 1.75 (q, *J* = 6.0 Hz, 1H), 1.49 – 1.19 (m, 38H), 0.89 (t, *J* = 6.8 Hz, 7H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 159.1, 142.6, 114.0, 113.0, 83.6, 81.5, 70.7, 38.0, 32.0 (2x), 31.4, 30.1, 29.8, 29.7 (3x) 29.4, 29.4, 26.9, 22.8, 22.7, 21.2, 14.2. HRMS (ESI$^+$): m/z calcd for $C_{30}H_{50}O$: 426.3862; found: 426.3829 $[M]^+$, diff = 7.76 ppm.



Compound 4: A mixture of compound 3 (2.13 g, 5.0 mmol), 1,4-dibromo-2,5-diiodobenzene (1.22 g, 2.5 mmol), $Pd(PPh_3)_2Cl_2$ (140 mg, 0.2 mmol), and CuI (76 mg, 0.4 mmol) was added to the dry and degassed flask filled with THF (25 mL) and diisopropylamine (DIPA) (5 mL). The reaction mixture was warm up to 60 °C and stirred for 15 hours. Afterward, the mixture was cooled

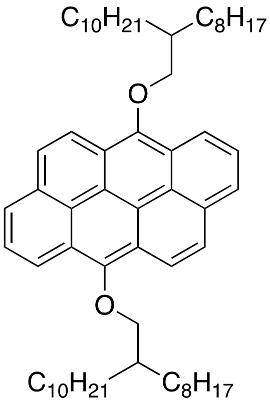
to room temperature, and filtered through the pad of silica. The residue was diluted with CH_2Cl_2 (50 mL). The mixture was subjected to washing with 10% aqueous NH_4OH, water, and brine. The organic phase was dried using $MgSO_4$, filtered, and evaporated under reduced pressure. The remaining residue was purified using silica gel column chromatography with a hexanes/DCM (9/1) solvent system. This purification process yielded the compound 4 (1.90 g, 70%) as a pale-yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.75 (s, 2H), 6.65 (d, J = 0.9 Hz, 4H), 3.84 (d, J = 5.6 Hz, 4H), 2.54 (s, 12H), 1.77 (q, J = 6.0 Hz, 3H), 1.50 – 1.20 (m, 79H), 0.90 (td, J = 7.0, 1.1 Hz, 12H).

^{13}C NMR (126 MHz, $CDCl_3$) δ = 159.6, 142.8, 135.7, 126.6, 122.9, 114.2, 113.2, 95.1, 93.8, 70.7, 37.9, 31.9, 31.3, 30.0, 29.7 (3x), 29.6, 29.4 (2x), 26.8, 22.7, 21.6, 14.2.

HRMS (ESI$^+$): m/z calcd for $C_{66}H_{100}O_2Br_2$: 1082.6090; found: 1082.6108 [M]$^+$, diff = 1.65 ppm.

Compound 5 was prepared according to a previously reported method.[2]



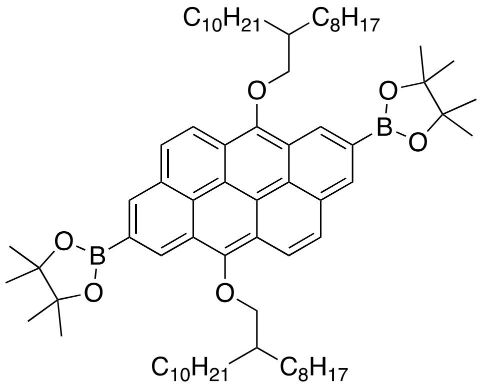
Compound 6: A dry round bottom flask was charged with a magnetic stir bar, compound **5** (5.14 g, 5.00 mmol), Pd(dppf)Cl_2 (182 mg, 0.25 mmol) and $NaBH_4$ (1.29 g, 34.0 mmol). The flask was degassed using a flow of nitrogen in 10 mins. Dry THF (300 mL) and *N,N,N',N'*-tetramethylethylenediamine (3.95 g, 34.0 mmol, 5.1 mL) were added to the mixture under nitrogen. The reaction mixture was heated to 60 °C and stirred for 12 hours. After cooling down to the ambient temperature, the mixture was filtered to remove the insoluble materials. A 1 M aqueous solution of hydrogen chloride (100 mL) was added to the filtrate. Organic materials were extracted with dichloromethane, washed with brine, dried over sodium sulfate and concentrated under vacuum. The crude material was dissolved in

minimum amount of hot chloroform, precipitated in cold methanol and filtered. Purification by silica gel column chromatography (CH_2Cl_2/hexanes 50:50 v/v) afforded compound **6** as a yellow solid (3.83 g, 88%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.77 (dd, *J* = 8.1, 1.2 Hz, 2H), 8.47 (d, *J* = 9.3 Hz, 2H), 8.23 – 8.19 (m, 2H), 8.15 (dd, *J* = 8.1, 7.3 Hz, 2H), 8.08 (d, *J* = 9.4 Hz, 2H), 4.25 (d, *J* = 5.7 Hz, 4H), 2.20 (p, *J* = 6.1 Hz, 2H), 1.85 (dt, *J* = 15.4, 6.7 Hz, 5H), 1.69 (dq, *J* = 13.8, 7.0 Hz, 4H), 1.58 – 1.46 (m, 11H), 1.41 – 1.26 (m, 48H), 0.95 – 0.84 (m, 12H).

^{13}C NMR (126 MHz, $CDCl_3$) δ = 149.4, 131.8, 127.9, 125.8, 125.6, 124.2, 123.9, 122.3, 122.2, 120.5, 120.4, 79.2, 39.8, 32.0 (2x), 31.5, 30.3, 29.8 (4x), 29.5 (2x), 27.2, 22.8 (2x), 14.2 (2x).

HRMS (ESI$^+$): m/z calcd for $C_{62}H_{92}O_2$: 868.7092; found: 868.7055 [M]$^+$, diff = 4.2 ppm.



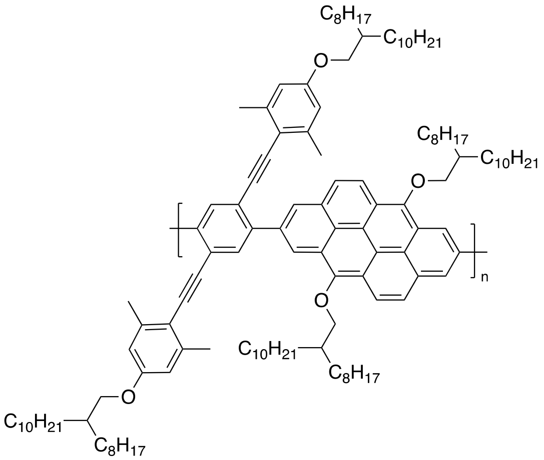
Compound 7: A dry flask was charged with Compound **6** (3.467 g, 4 mmol), $[Ir(cod)OMe]_2$ (132 mg, 0.2 mmol), bis(pinacolato)diboron (2.032 mg, 8.0 mmol) and 4,4'-di-*tert*-butyl-2,2'-bipyridine (dtbpy; 214 mg, 0.80 mmol). The flask was degassed with a flow of nitrogen in 20 min before it was charged with cyclohexane (50 mL) and heated to 80 °C. After 12 hours, the reaction mixture was cooled down and was concentrated under vacuum. The residue was dissolved in dichloromethane, washed with water and dried over sodium sulfate. Purification by silica gel column chromatography (100 % CH_2Cl_2) afforded 3.63 g (81%) of compound **7** as a yellow powder.

^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.29 (d, *J* = 0.9 Hz, 2H), 8.60 (d, *J* = 0.8 Hz, 2H), 8.46 (d, *J* = 9.3 Hz, 2H), 8.09 (d, *J* = 9.4 Hz, 2H), 4.29 (d, *J* = 5.5 Hz, 4H), 2.22 (hept, *J* = 6.1 Hz, 2H), 1.97 – 1.86

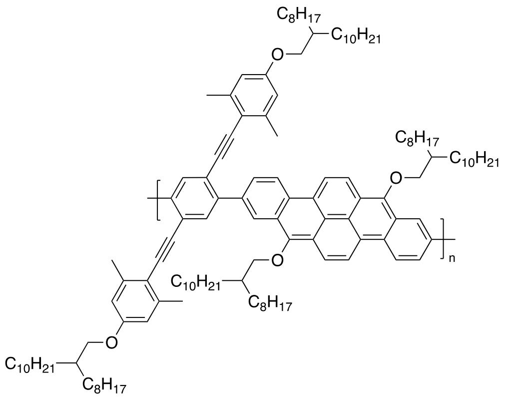
(m, 4H), 1.78 – 1.67 (m, 4H), 1.63 – 1.51 (m, 11H), 1.49 – 1.39 (m, 7H), 1.39 – 1.23 (m, 33H), 0.90 (dd, *J* = 9.9, 4.8 Hz, 14H).

^{13}C NMR (126 MHz, $CDCl_3$) δ = 149.8, 131.1, 129.2, 128.1, 127.9, 125.6, 125.1, 122.4, 122.3, 121.1, 84.1, 79.6, 39.8, 32.0 (2x), 31.6, 30.2, 29.8 (2x), 29.7 (2x), 29.5, 29.4, 27.2, 25.1, 22.7 (2x), 14.2, 14.1.

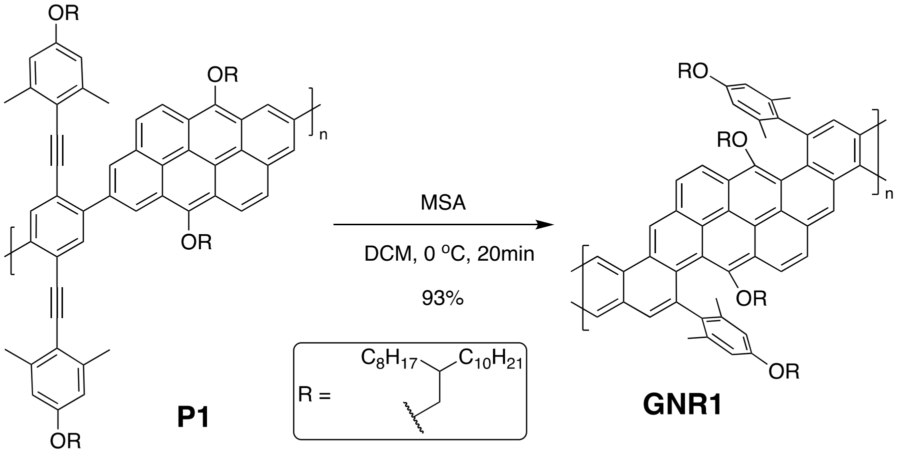
HRMS (ESI$^+$): m/z calcd for $C_{74}H_{114}O_6B_2$: 1120.88182; found: 1120.8865 [M]$^+$, diff = 4.1 ppm.



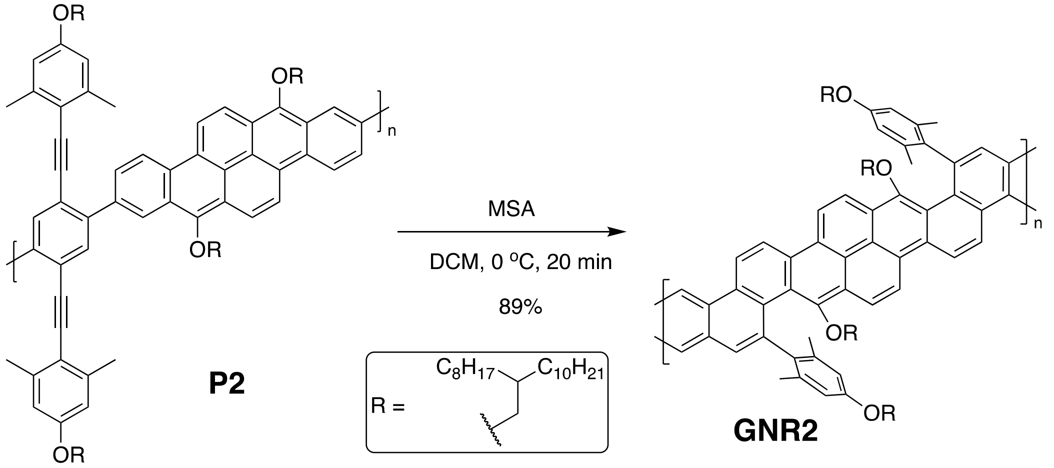
P1: A round bottom flask was charged with monomer 4 (1.121 g, 1.00 mmol), monomer 7 (1.085 g, 1.00 mmol), $Pd(PPh_3)_4$ (23 mg, 0.02 mmol) and a magnetic stir bar. The flask was nitrogen purging for 15 minutes. The nitrogen purged solution of Aliquant 336 (0.1 mL) in toluene (20 mL) was added to the reaction mixture. The nitrogen purged solution of K_2CO_3 (2M, 2.5 mL, 5.0 mmol) was added to the reaction mixture and the mixture was warmed to 90 °C and stirred for 65 hours. Afterwards, the mixture was cooled down and precipitated to of cold methanol (50 mL) and filtered. The resulting precipitate was filtered under vacuum and washed with methanol. The low weight oligomers were removed by washing the residue with methanol and hexanes, using Soxhlet apparatus and the polymer was extracted with chloroform by removing the remain of catalyst by using the same apparatus. The extraction afforded 1.525 g (85%) of **P1** as a yellow solid.



P2: The same procedure was used for the synthesis and extraction of **P1** was applied for the synthesis of **P2**. 1 mmol of the compound **8** (1.147 g) was used for this reaction. This reaction afforded **P2** as a yellow solid (1.657 g, 91%).



GNR1: A 250 ml flame dried round bottom flask was charged with a magnetic stir bar, **P1** (897 mg, 0.5 mmol) and nitrogen purged DCM (80 mL). The mixture was cooled down to 0 °C during the purge of nitrogen. Then, methanesulfonic acid (MSA) (144 mg, 0.1 mL) was added dropwise and the mixture was stirred for 20 minutes. The excess of MSA was quenched with saturated solution of $NaHCO_3$ (40 mL) and the organic phase was extracted and dried over anhydrous sodium sulfate and filtered. The solvent was removed under reduced pressure to afford **GNR1** as a blue solid (834 mg, 93%).



GNR2: Same procedure that was used for synthesis and extraction of **GNR1** was used for the benzannulation of **P2** (910 mg, 0.5 mmol) to afford **GNR2** as a purple solid (810 mg, 89%).

NMR Spectra

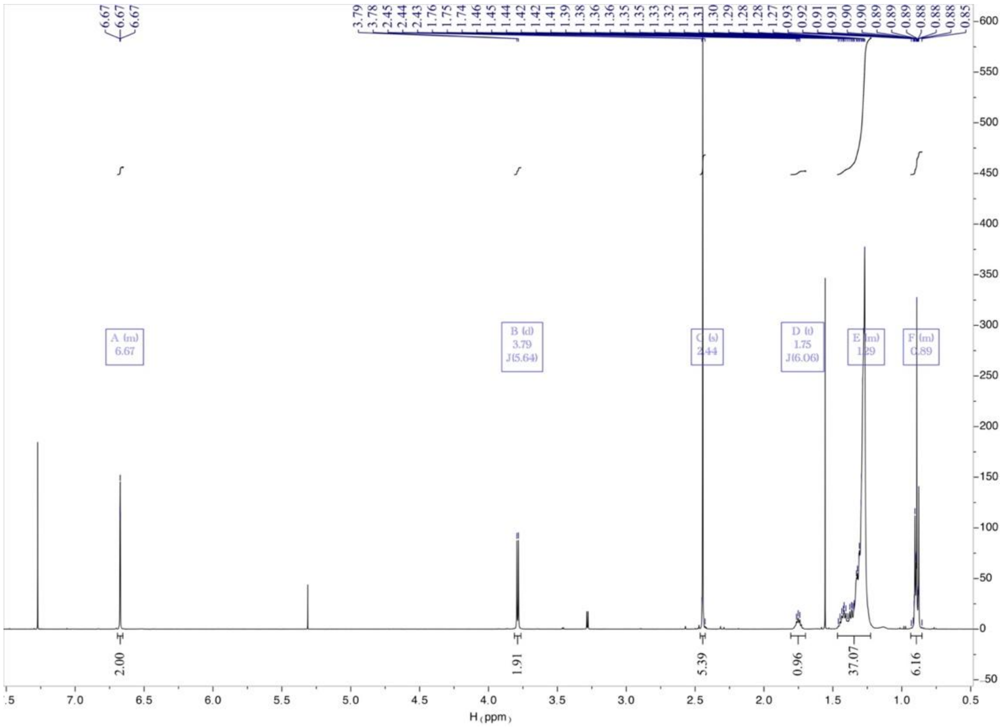


Fig. S1: ^{1}H NMR spectrum of compound **1** in $CDCl_3$ at 500 MHz.

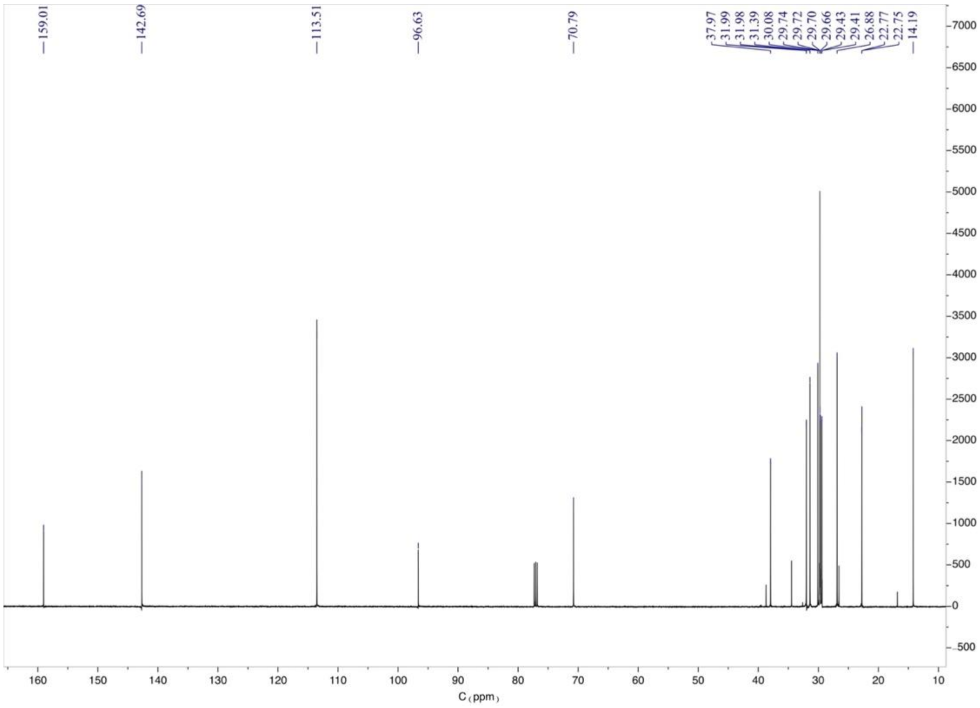


Fig. S2: ^{13}C NMR spectrum of compound **1** in $CDCl_3$ at 126 MHz.

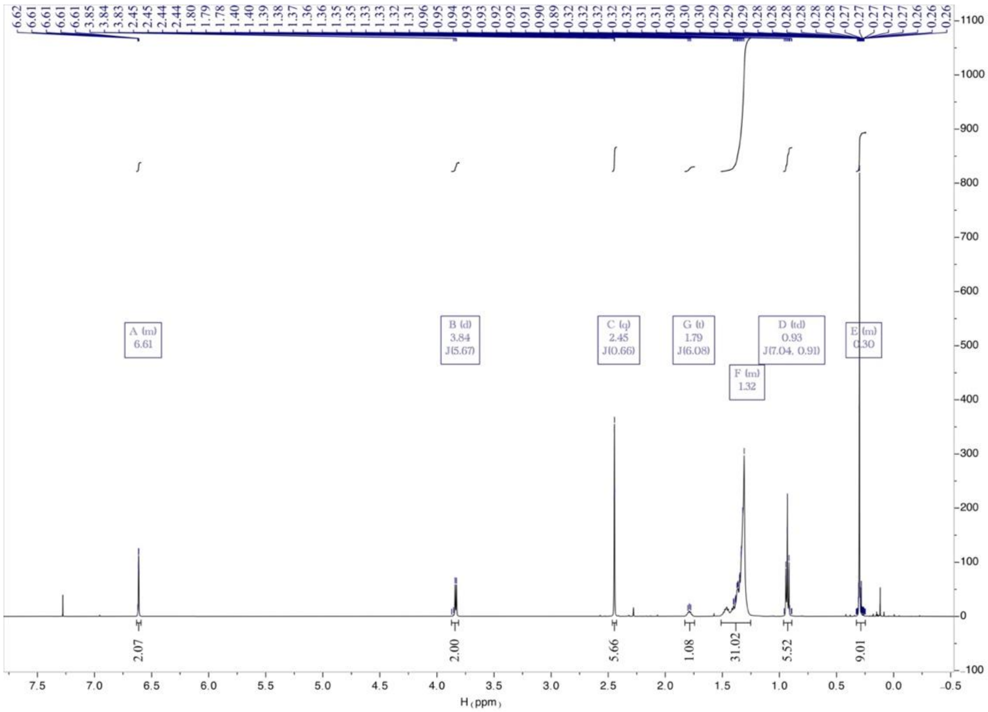


Fig. S3: ^{1}H NMR spectrum of compound **2** in $CDCl_3$ at 500 MHz.

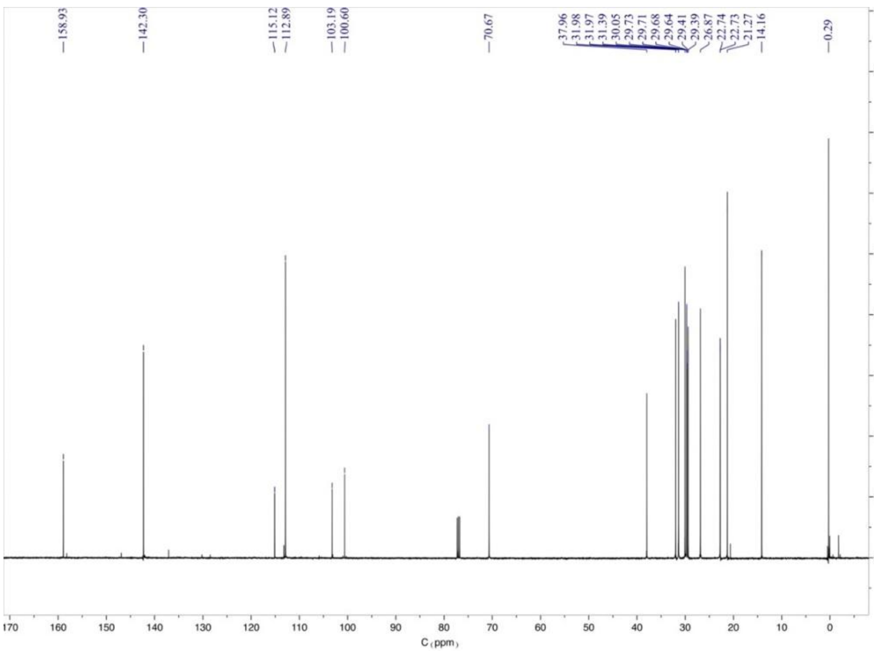


Fig. S4: ^{13}C NMR spectrum of compound **2** in $CDCl_3$ at 126 MHz.

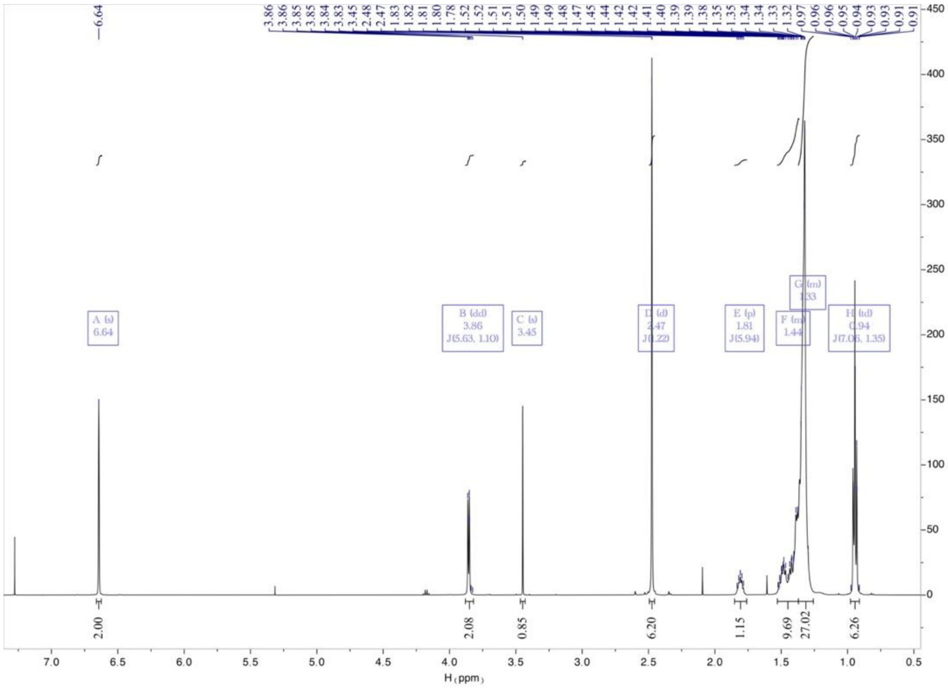


Fig. S5: ^{1}H NMR spectrum of compound **3** in $CDCl_3$ at 500 MHz.

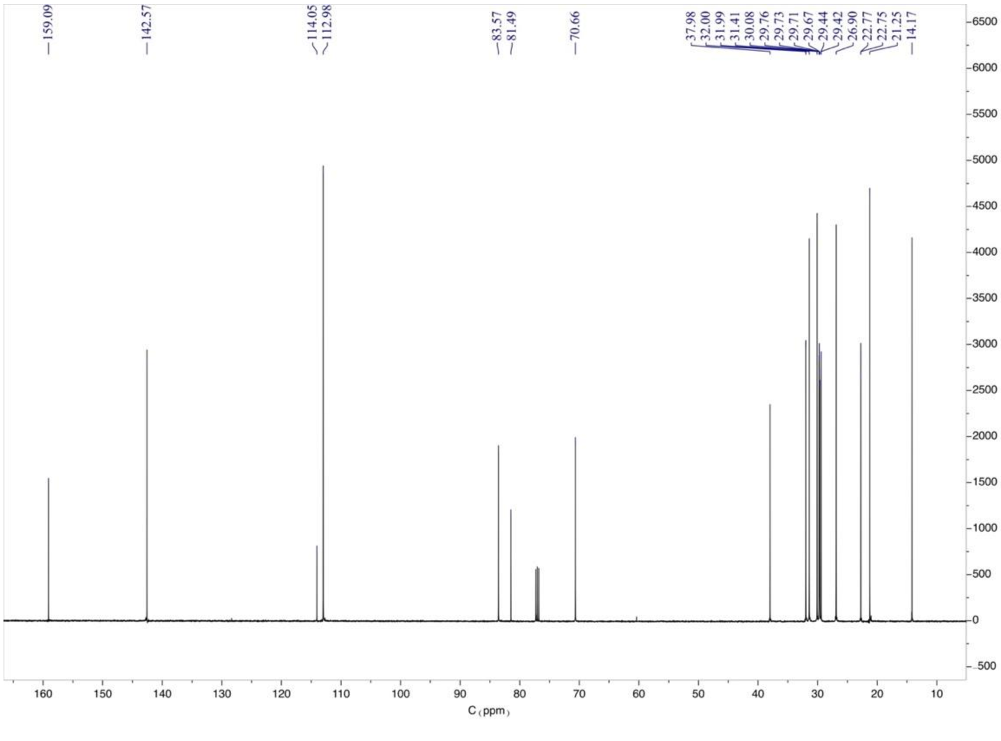


Fig. S6: ^{13}C NMR spectrum of compound **3** in $CDCl_3$ at 126 MHz.

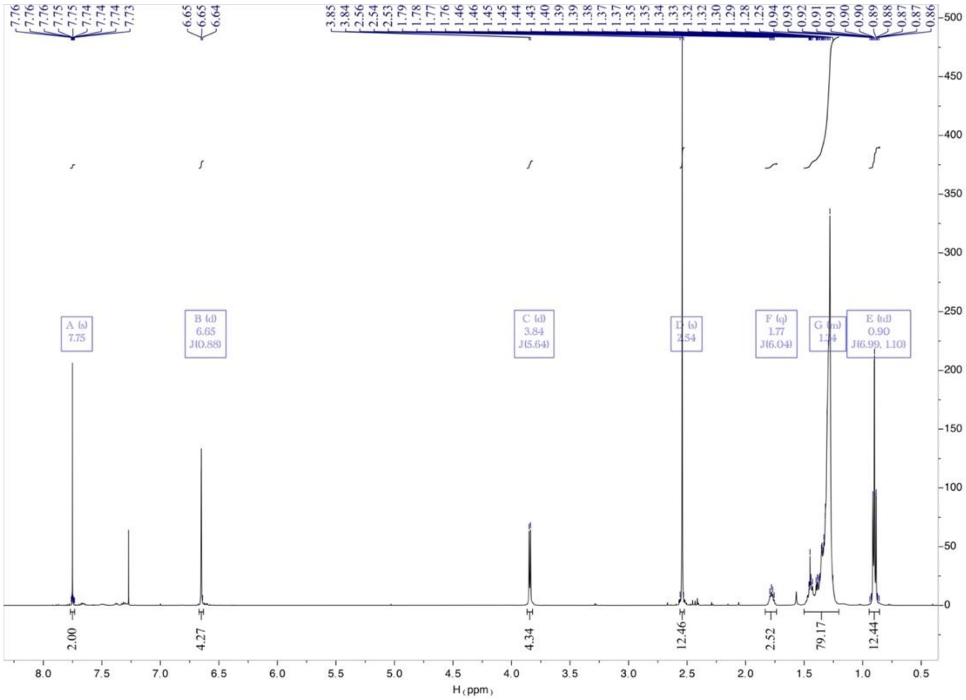


Fig. S7: ^{1}H NMR spectrum of compound **4** in CDCl$_3$ at 500 MHz.

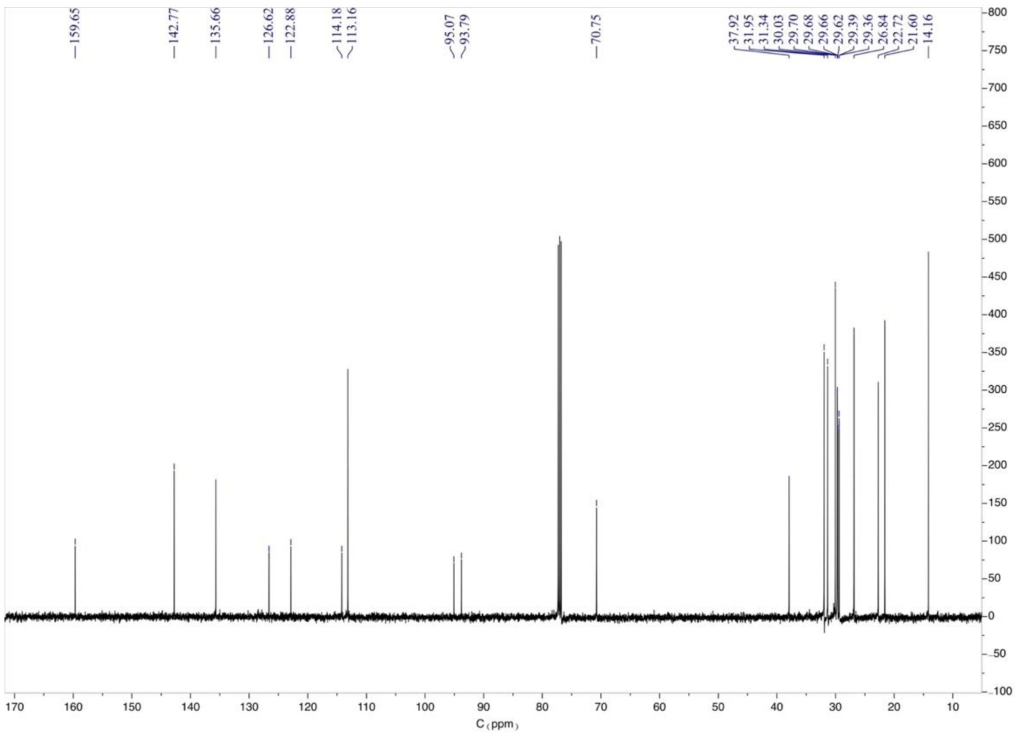


Fig. S8: ^{13}C NMR spectrum of compound **4** in CDCl$_3$ at 126 MHz.

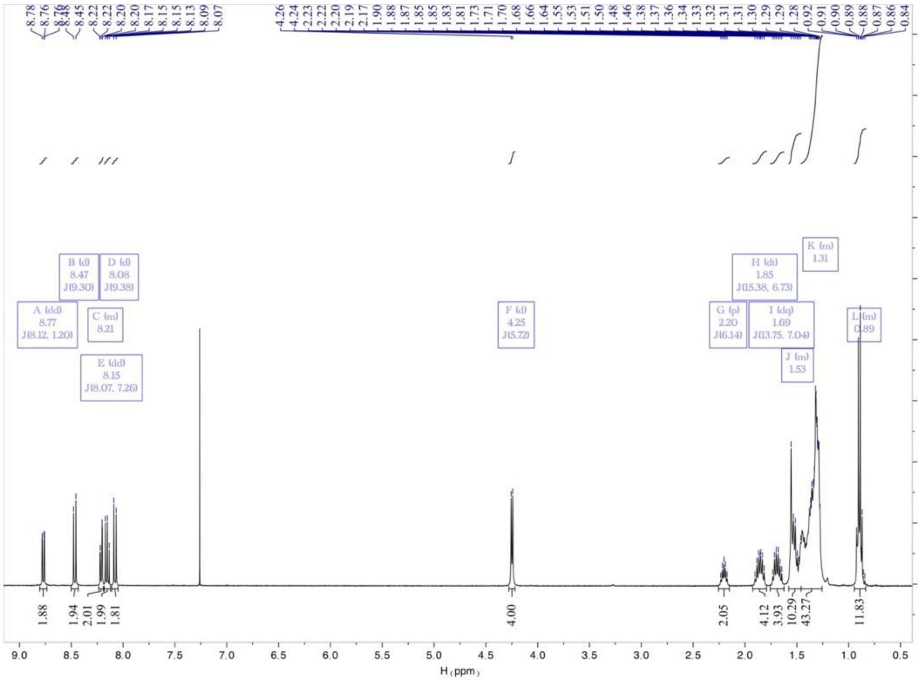


Fig. S9: ^{1}H NMR spectrum of compound **6** in $CDCl_3$ at 400 MHz.

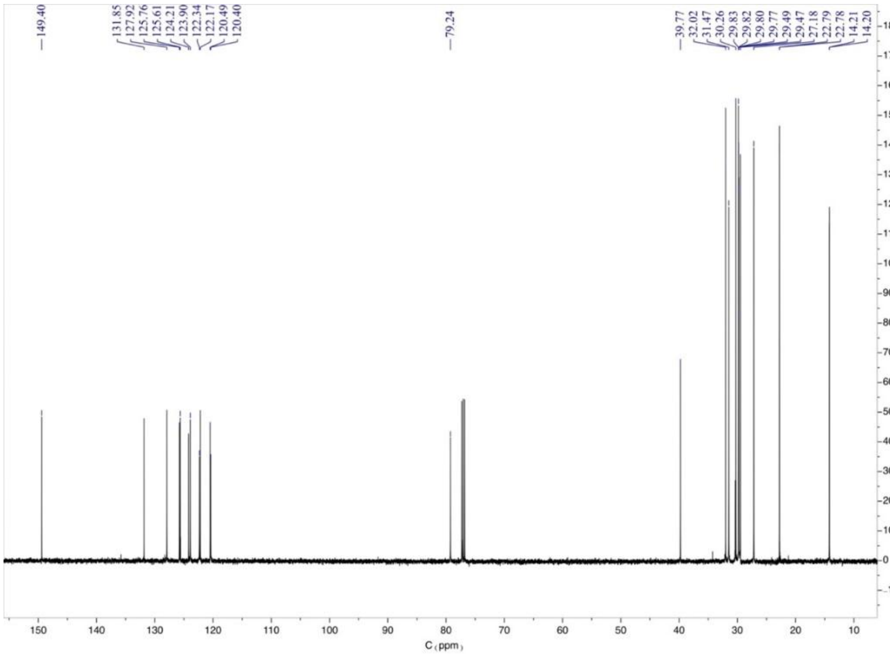


Fig. S10: ^{13}C NMR spectrum of compound **6** in $CDCl_3$ at 126 MHz.

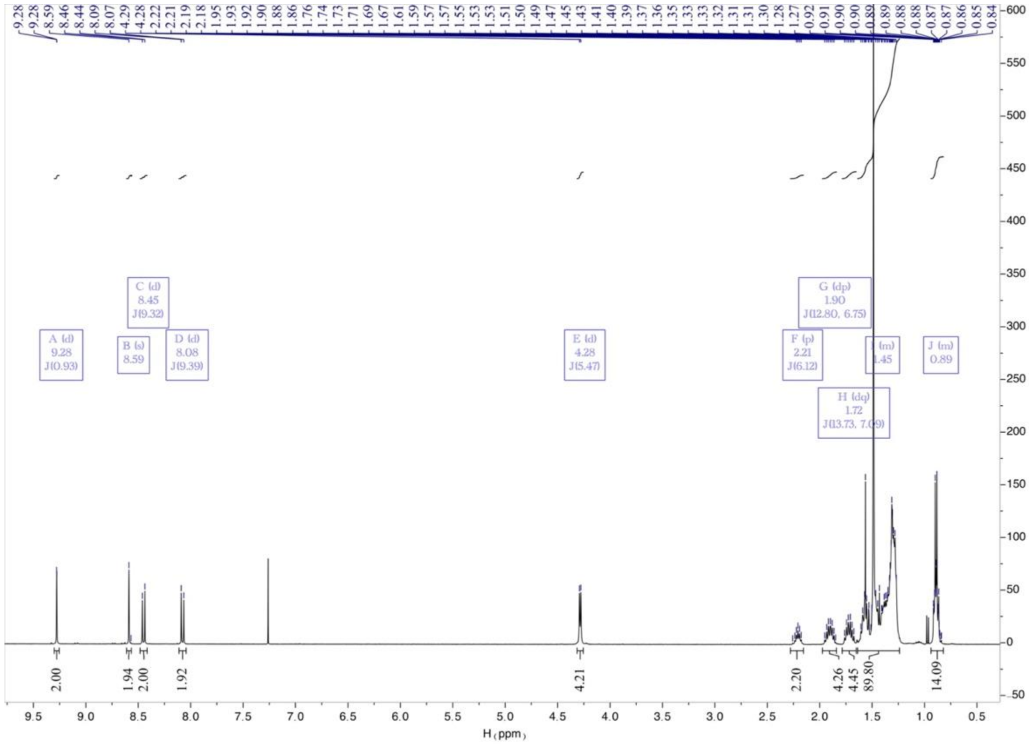


Fig. S11: ^{1}H NMR spectrum of compound **7** in CDCl$_3$ at 500 MHz.

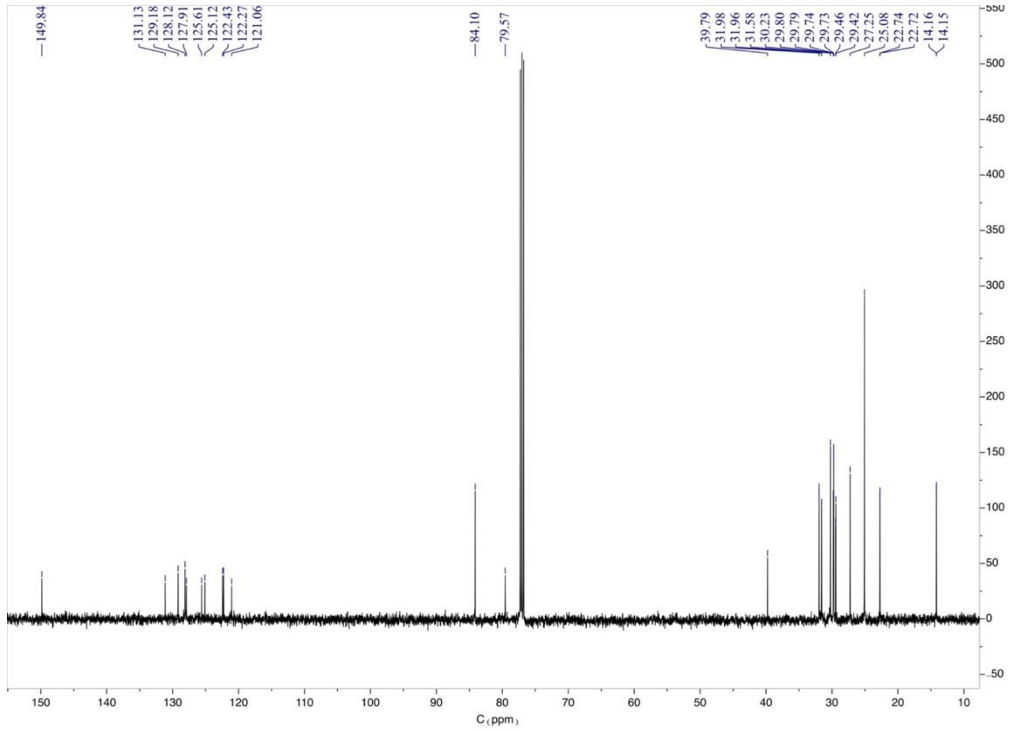


Fig. S12: ^{13}C NMR spectrum of compound **7** in CDCl$_3$ at 126 MHz.

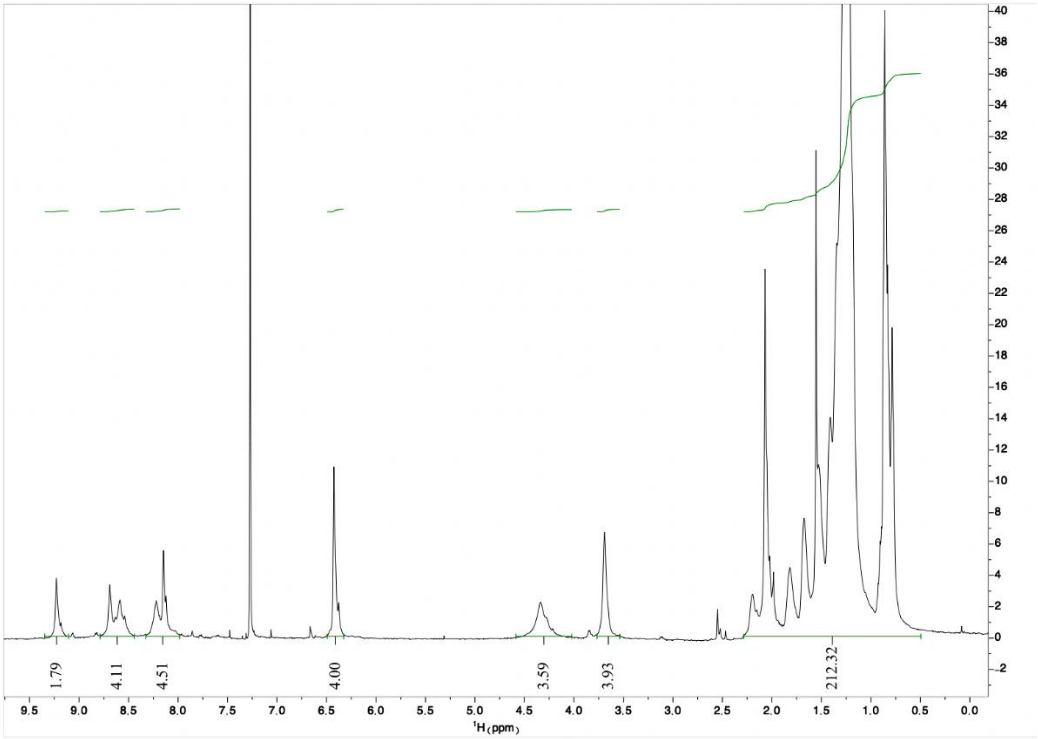


Fig. S13: ^{1}H NMR spectrum of **P1** in $CDCl_3$ at 500 MHz.

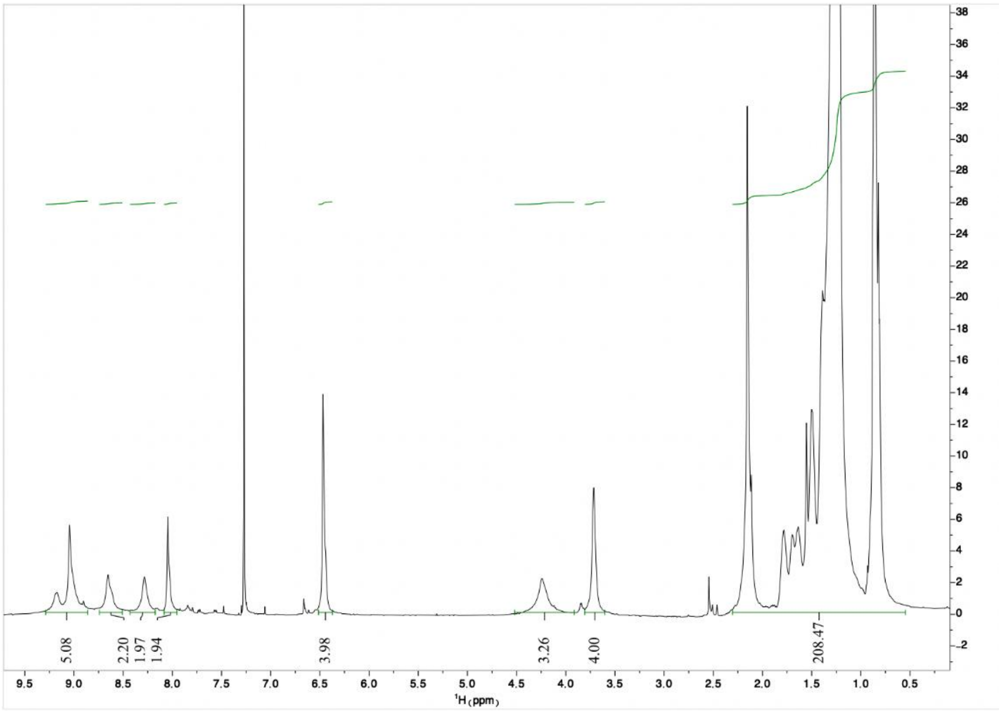


Fig. S14: ^{1}H NMR spectrum of **P2** in $CDCl_3$ at 500 MHz.

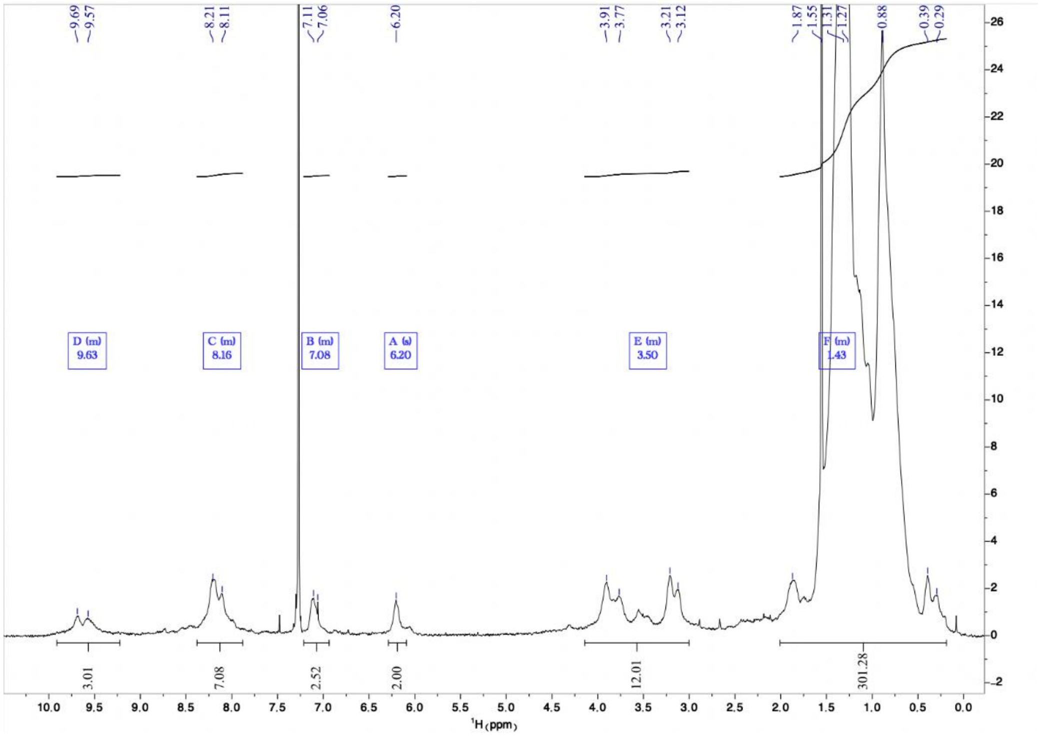


Fig. S15: ^{1}H NMR spectrum of **GNR1** in $CDCl_3$ at 500 MHz.

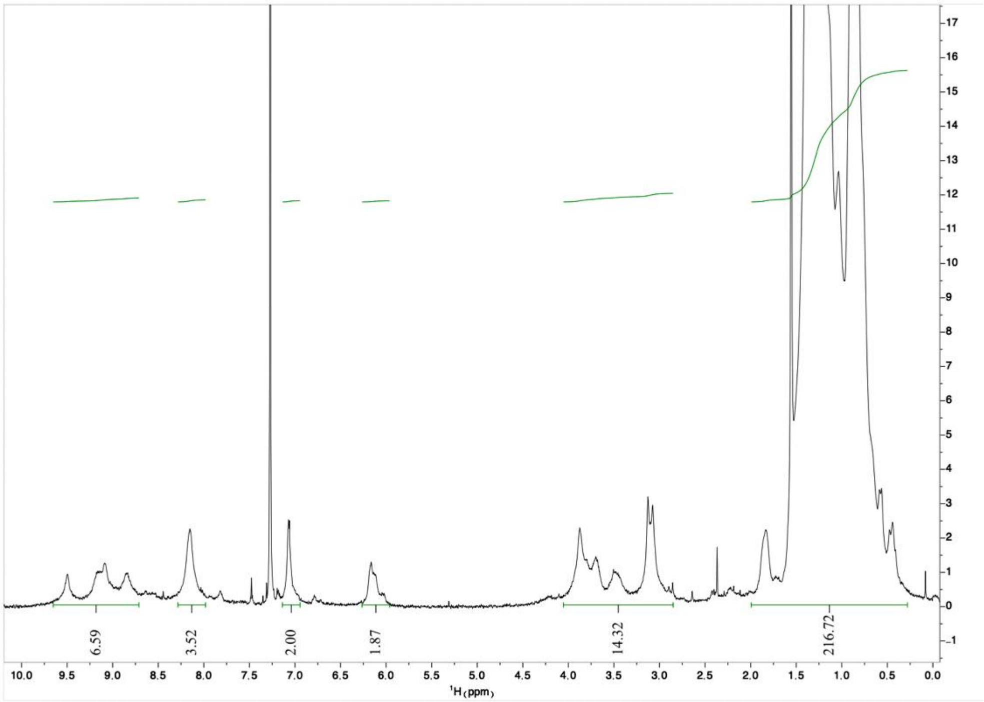


Fig. S16: ^{1}H NMR spectrum of **GNR2** in $CDCl_3$ at 500 MHz.

FT-IR spectra

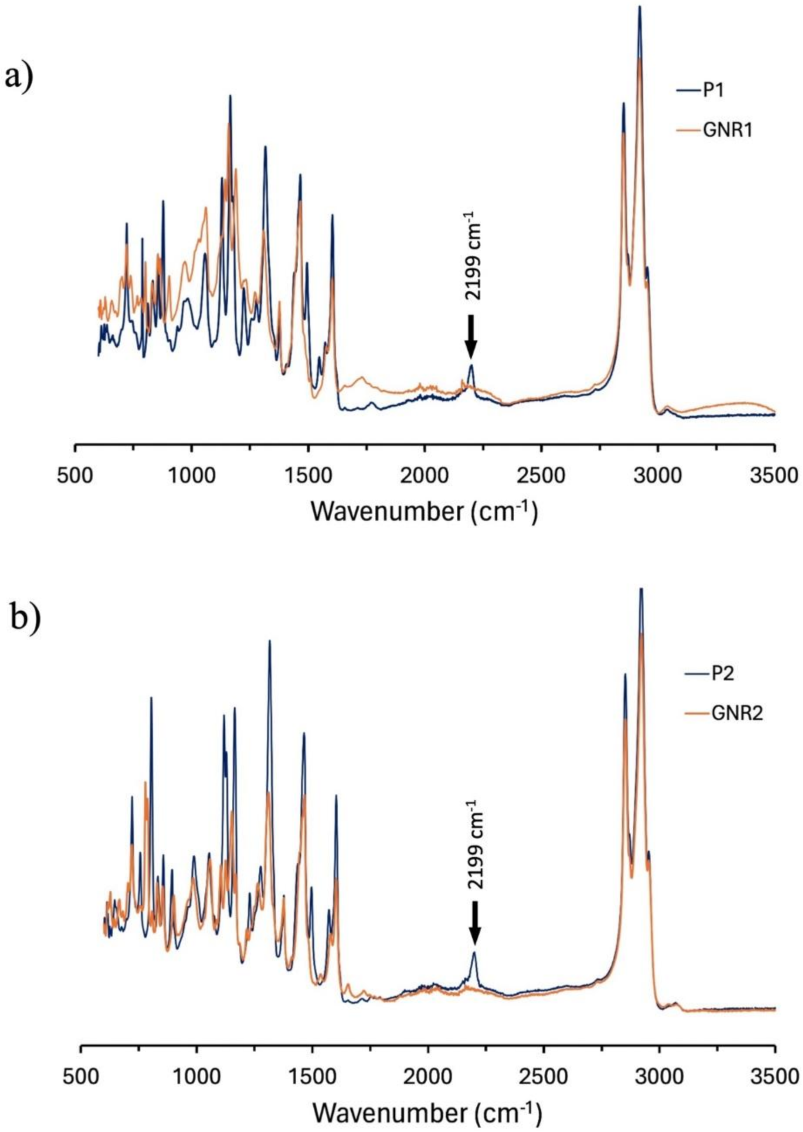


Fig. S17: FT-IR spectra of a) **P1** and **GNR1**, b) **P2** and **GNR2**.

DSC plots

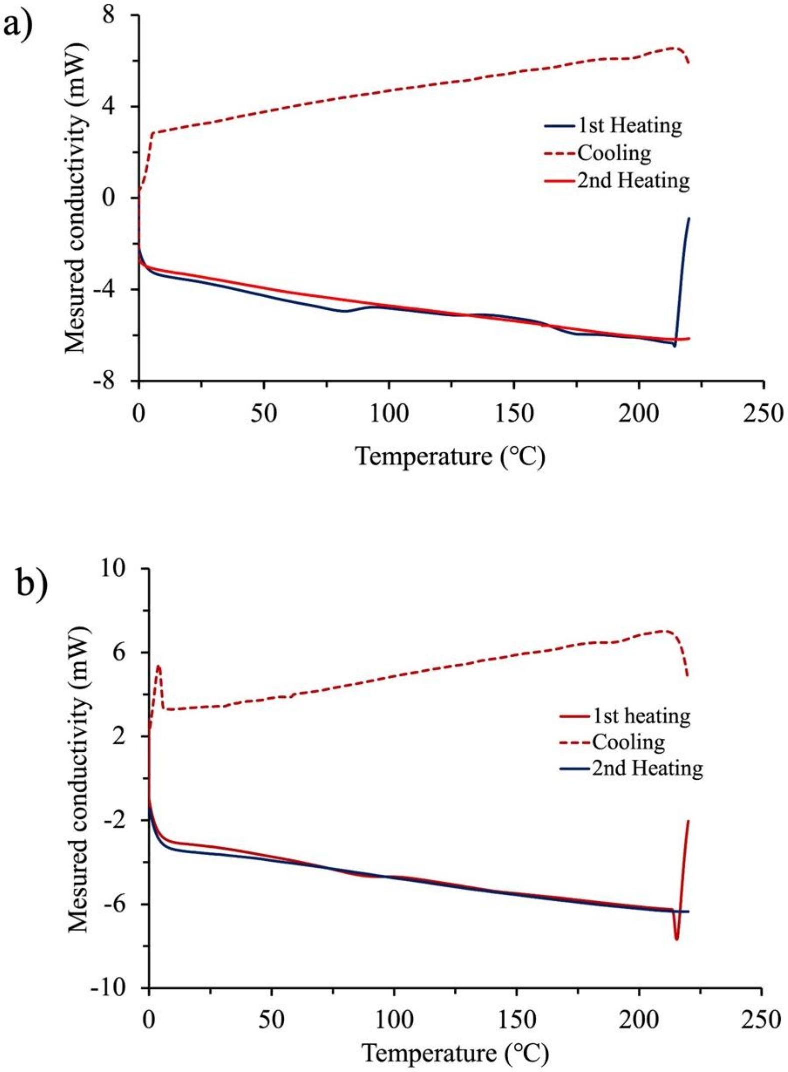


Fig. S18. a) Differential scanning calorimetry plots of a) **GNR1** and b) **GNR2**.

TGA graph

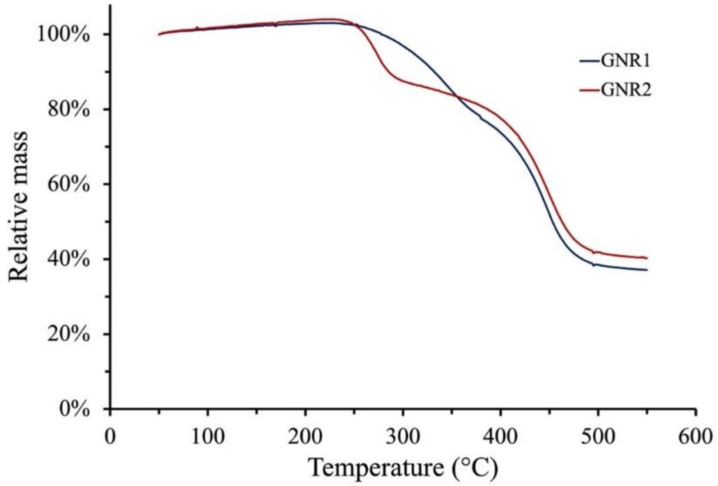


Fig. S19. Thermogravimetric analysis curves of **GNR1** and **GNR2** under nitrogen at a heating rate of 10 °C/minute.

Cyclic voltammogram

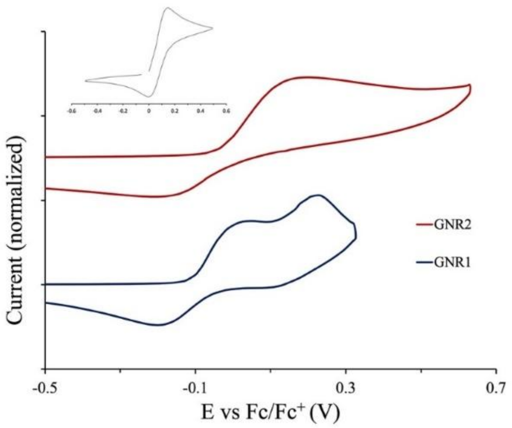
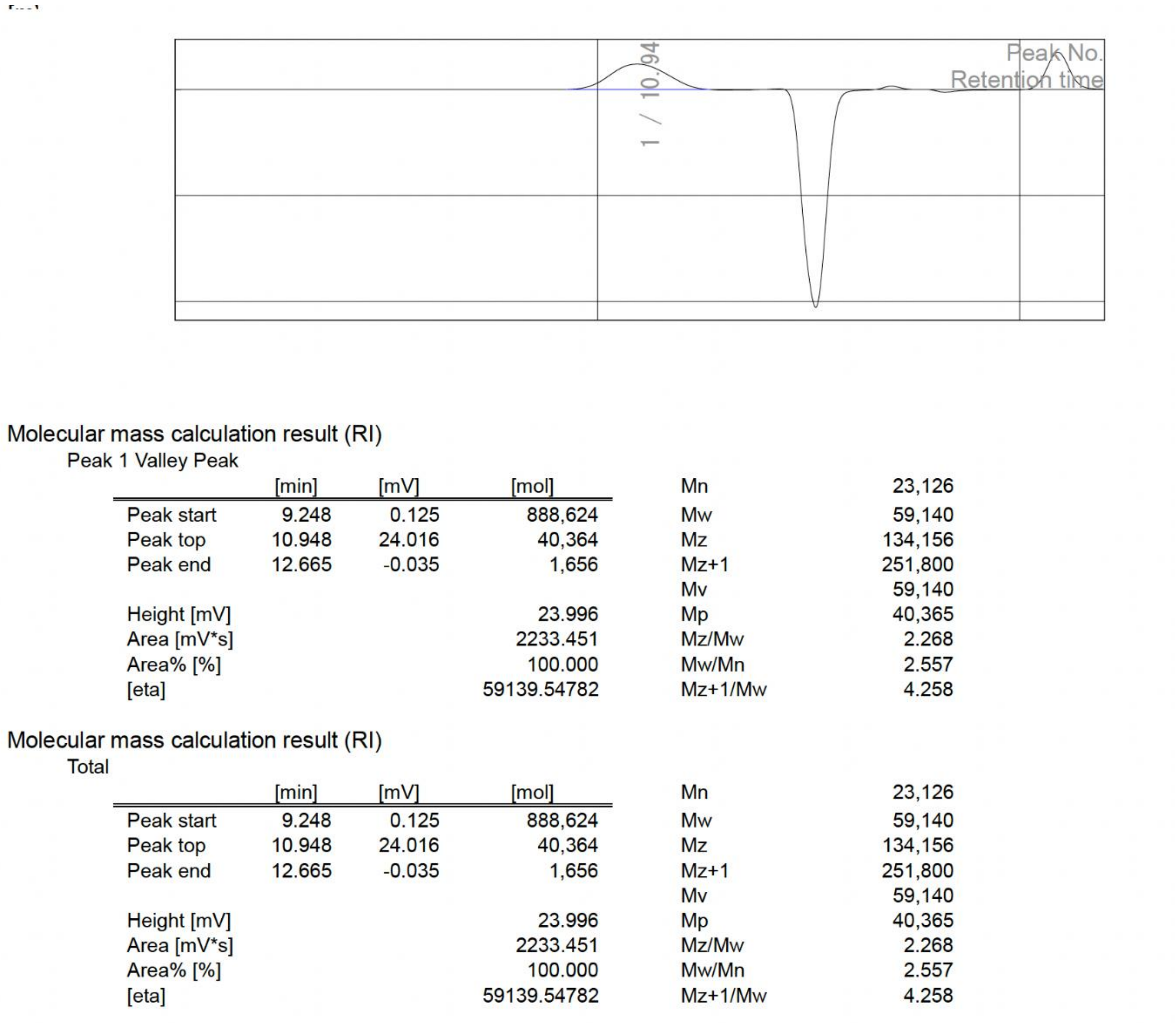


Fig. S20. Cyclic Voltammetry of **GNR1** and **GNR2** in acetonitrile solution with 0.1M [Bu_4N][BF_4] as the supporting electrolyte with a scan rate of 50 mV·s^{-1} in the thin film state. Platinum wires were used as working and counter electrodes, and $Ag/AgNO_3$ in acetonitrile was used as the reference electrode.

Size exclusion chromatography



Molecular mass calculation result (RI)

Peak 1 Valley Peak

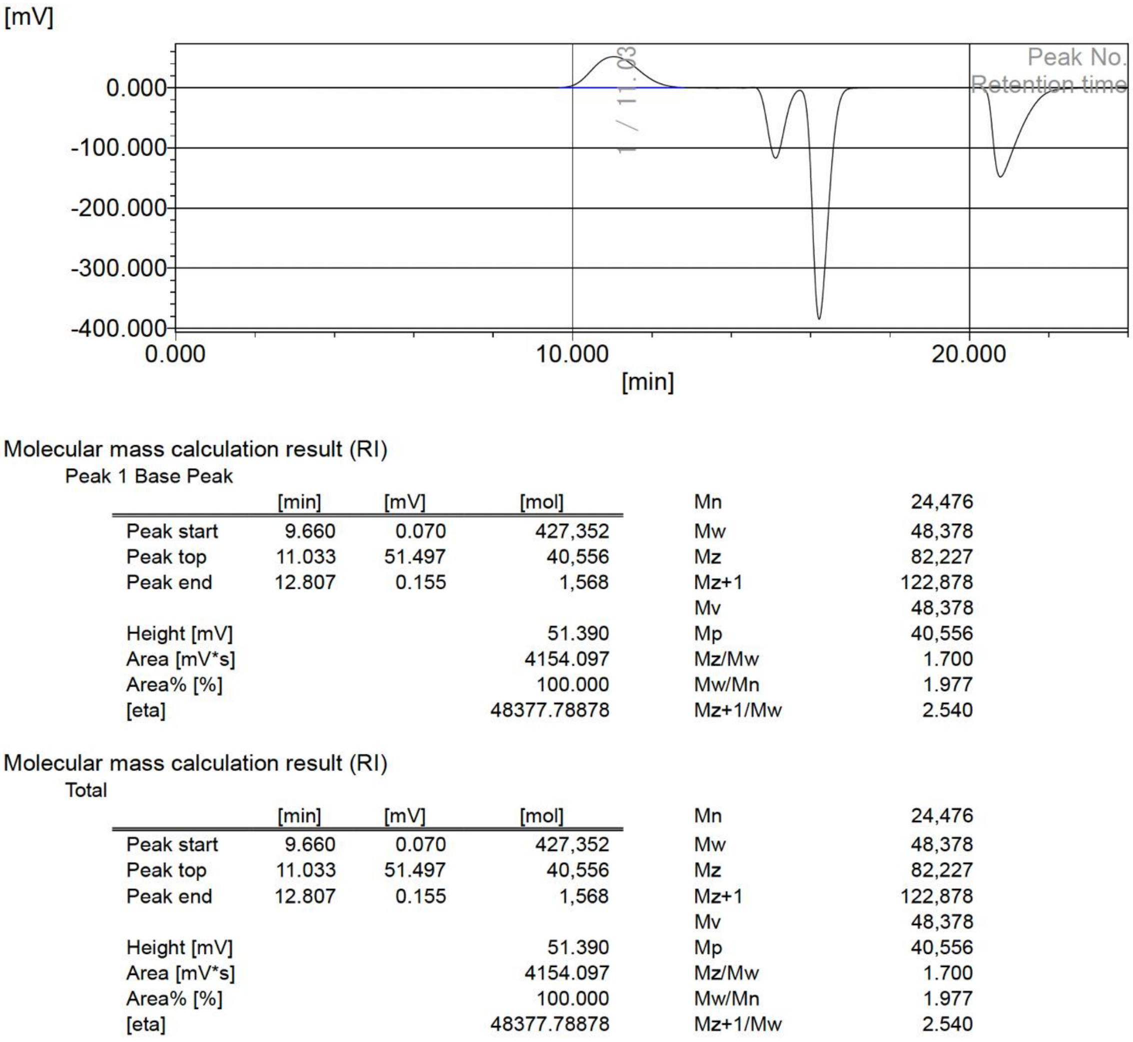
	[min]	[mV]	[mol]		
Peak start	9.248	0.125	888,624	Mn	23,126
Peak top	10.948	24.016	40,364	Mw	59,140
Peak end	12.665	-0.035	1,656	Mz	134,156
				Mz+1	251,800
				Mv	59,140
Height [mV]			23.996	Mp	40,365
Area [mV*s]			2233.451	Mz/Mw	2.268
Area% [%]			100.000	Mw/Mn	2.557
[eta]			59139.54782	Mz+1/Mw	4.258

Molecular mass calculation result (RI)

Total

	[min]	[mV]	[mol]		
Peak start	9.248	0.125	888,624	Mn	23,126
Peak top	10.948	24.016	40,364	Mw	59,140
Peak end	12.665	-0.035	1,656	Mz	134,156
				Mz+1	251,800
				Mv	59,140
Height [mV]			23.996	Mp	40,365
Area [mV*s]			2233.451	Mz/Mw	2.268
Area% [%]			100.000	Mw/Mn	2.557
[eta]			59139.54782	Mz+1/Mw	4.258

Fig. S21. Size exclusion chromatography (SEC) report for polymer **P1**. This involved utilizing 1,2,4-trichlorobenzene as the eluent and employing polystyrene as the standard for measurements at 110 °C.



Molecular mass calculation result (RI)
Peak 1 Base Peak

	[min]	[mV]	[mol]
Peak start	9.660	0.070	427,352
Peak top	11.033	51.497	40,556
Peak end	12.807	0.155	1,568
Height [mV]			51.390
Area [mV*s]			4154.097
Area% [%]			100.000
[eta]			48377.78878

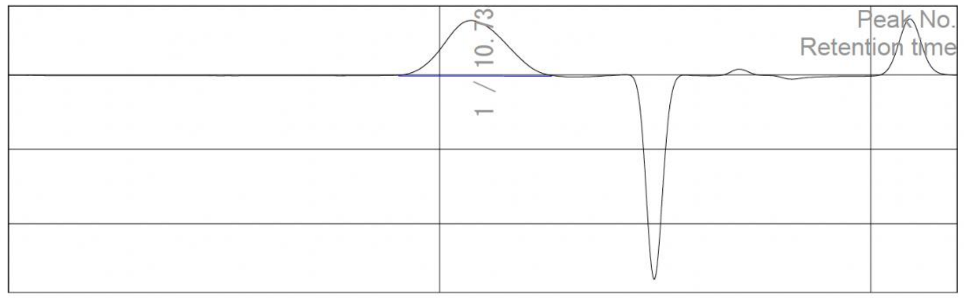
Mn	24,476
Mw	48,378
Mz	82,227
Mz+1	122,878
Mv	48,378
Mp	40,556
Mz/Mw	1.700
Mw/Mn	1.977
Mz+1/Mw	2.540

Molecular mass calculation result (RI)
Total

	[min]	[mV]	[mol]
Peak start	9.660	0.070	427,352
Peak top	11.033	51.497	40,556
Peak end	12.807	0.155	1,568
Height [mV]			51.390
Area [mV*s]			4154.097
Area% [%]			100.000
[eta]			48377.78878

Mn	24,476
Mw	48,378
Mz	82,227
Mz+1	122,878
Mv	48,378
Mp	40,556
Mz/Mw	1.700
Mw/Mn	1.977
Mz+1/Mw	2.540

Fig. S22. Size exclusion chromatography (SEC) report for **GNR1**. This involved utilizing 1,2,4-trichlorobenzene as the eluent and employing polystyrene as the standard for measurements at 110 °C.



Molecular mass calculation result (RI)

Peak 1 Valley Peak

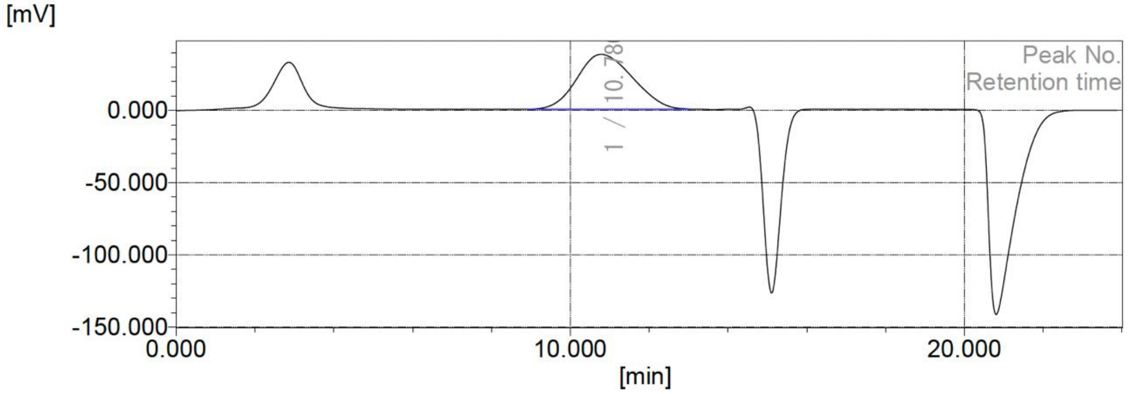
	[min]	[mV]	[mol]	Mn	27,587
Peak start	9.047	-0.055	1,398,005	Mw	86,286
Peak top	10.735	36.634	57,376	Mz	238,170
Peak end	12.598	-0.225	1,923	Mz+1	492,267
				Mv	86,286
Height [mV]			37.290	Mp	56,748
Area [mV*s]			3715.375	Mz/Mw	2.760
Area% [%]			100.000	Mw/Mn	3.128
[eta]			86286.15434	Mz+1/Mw	5.705

Molecular mass calculation result (RI)

Total

	[min]	[mV]	[mol]	Mn	27,587
Peak start	9.047	-0.055	1,398,005	Mw	86,286
Peak top	10.735	36.634	57,376	Mz	238,170
Peak end	12.598	-0.225	1,923	Mz+1	492,267
				Mv	86,286
Height [mV]			37.290	Mp	56,748
Area [mV*s]			3715.375	Mz/Mw	2.760
Area% [%]			100.000	Mw/Mn	3.128
[eta]			86286.15434	Mz+1/Mw	5.705

Fig. S23. Size exclusion chromatography (SEC) report for polymer **P2**. This involved utilizing 1,2,4-trichlorobenzene as the eluent and employing polystyrene as the standard for measurements at 110 °C.



Molecular mass calculation result (RI)

Peak 1 Base Peak

	[min]	[mV]	[mol]
Peak start	8.928	0.920	2,317,637
Peak top	10.780	38.921	60,355
Peak end	13.042	1.042	877
Height [mV]			37.946
Area [mV*s]			3707.778
Area% [%]			100.000
[eta]			81759.11199

Mn	27,741
Mw	81,759
Mz	216,385
Mz+1	495,545
Mv	81,759
Mp	57,115
Mz/Mw	2.647
Mw/Mn	2.947
Mz+1/Mw	6.061

Molecular mass calculation result (RI)

Total

	[min]	[mV]	[mol]
Peak start	8.928	0.920	2,317,637
Peak top	10.780	38.921	60,355
Peak end	13.042	1.042	877
Height [mV]			37.946
Area [mV*s]			3707.778
Area% [%]			100.000
[eta]			81759.11199

Mn	27,741
Mw	81,759
Mz	216,385
Mz+1	495,545
Mv	81,759
Mp	57,115
Mz/Mw	2.647
Mw/Mn	2.947
Mz+1/Mw	6.061

Fig. S24. Size exclusion chromatography (SEC) report for **GNR2**. This involved utilizing 1,2,4-trichlorobenzene as the eluent and employing polystyrene as the standard for measurements at 110 °C.

Charge transfer of device

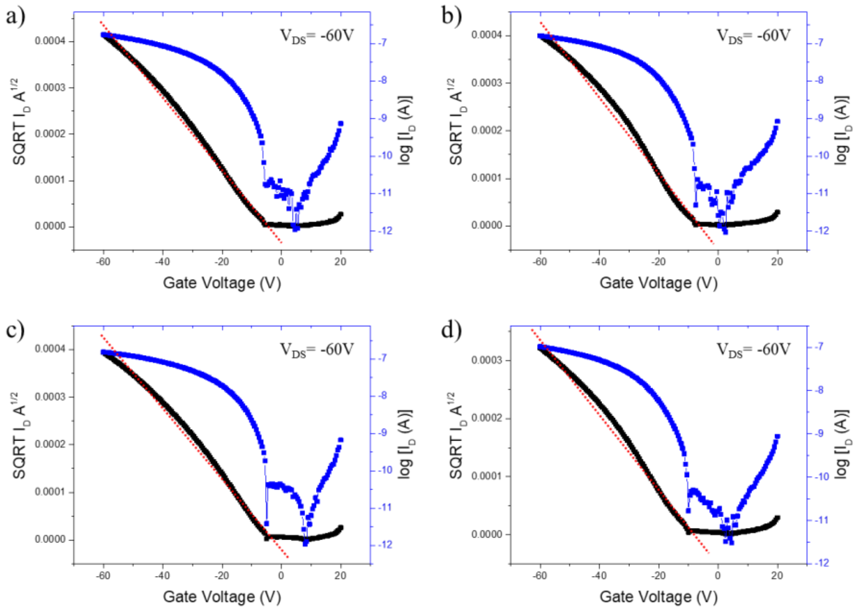


Fig. S25. Transfer curves of **GNR1** processed from a) toluene and c) 2-MeTHF, and **GNR2** processed from b) toluene and d) 2-MeTHF. The red dotted lines indicate the slopes used to calculate charge carrier mobility for each transfer curve.

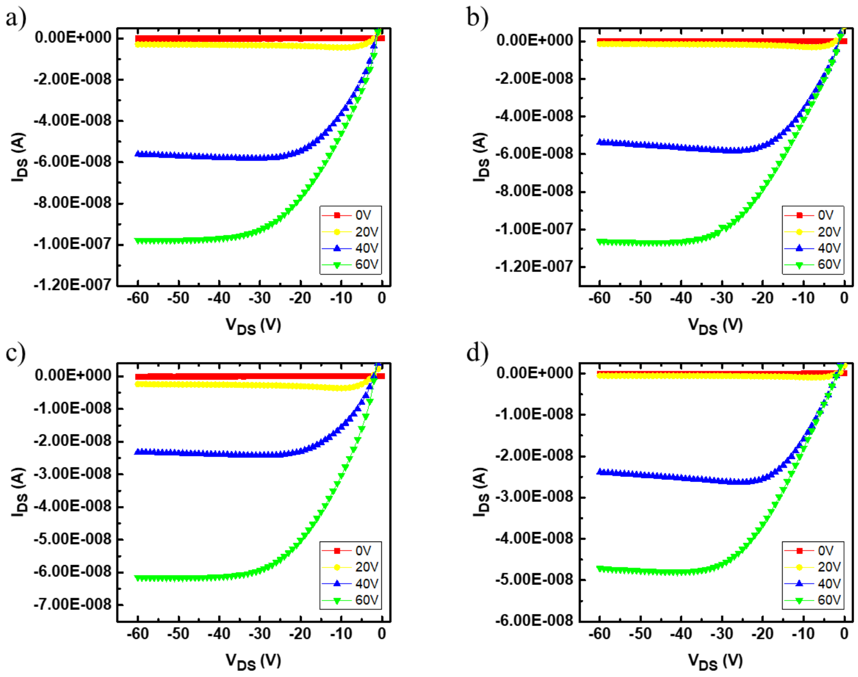


Fig. S26. Output curves of **GNR1** processed from a) toluene and c) 2-MeTHF, and **GNR2** processed from b) toluene and d) 2-MeTHF. The gate voltage was scanned from 0 to -60V with a step of -20V.

Atomic Force Microscopy (AFM)

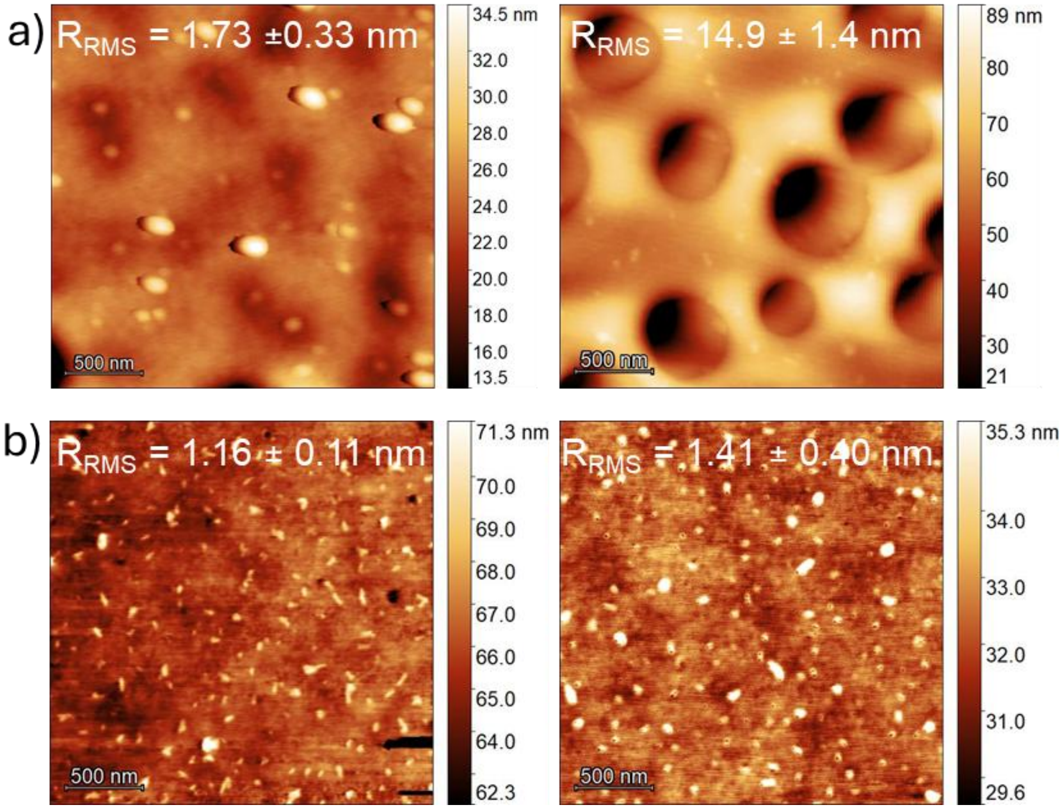


Figure S27. Atomic force microscopy (AFM) height images of a) **GNR1** processed from toluene (left) and 2-MeTHF (right), and b) **GNR2** processed from toluene (left) and 2-MeTHF (right). Size is 2.5 µm x 2.5 µm and scale bar is 500 nm.

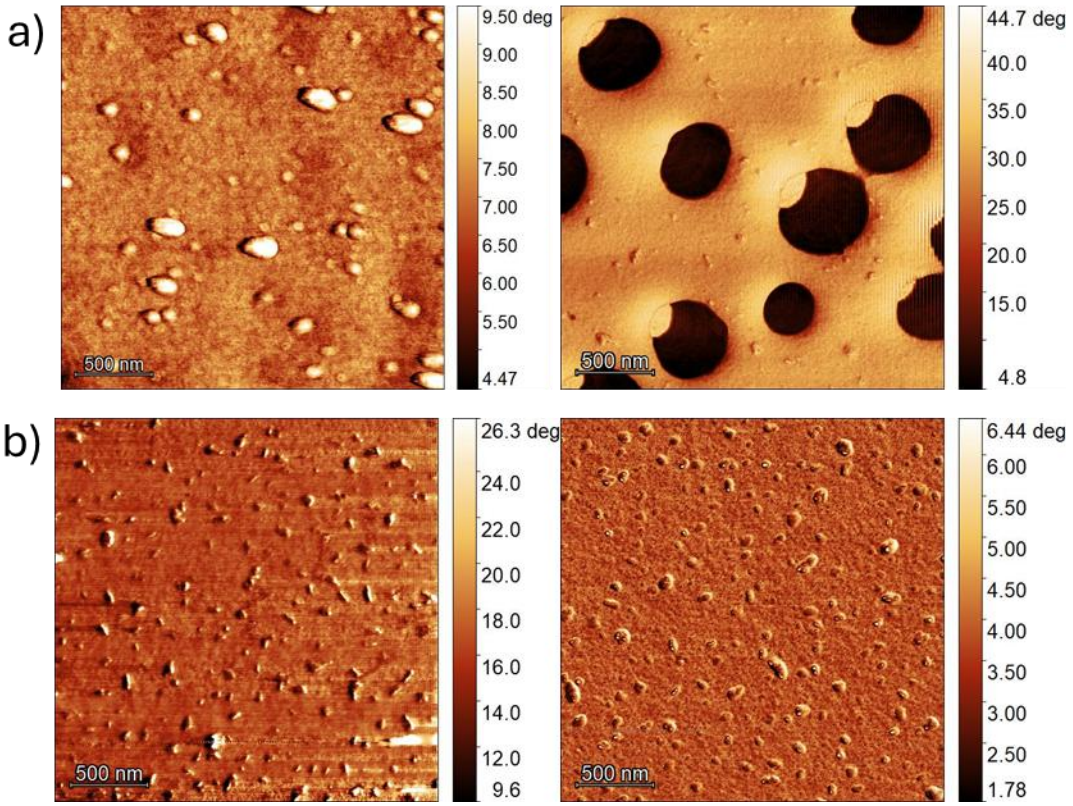


Figure S28. Atomic force microscopy (AFM) phase images of a) **GNR1** processed from toluene (left) and 2-MeTHF (right), and b) **GNR2** processed from toluene (left) and 2-MeTHF (right). Size is 2.5 μm x 2.5 μm and scale bar is 500 nm.

DFT Calculations

DFT calculations for the geometry optimization as well as frequency optimization of oligomers of **GNR1** and **GNR2** (two repeating units) were carried out with Gaussian 09 suites[2] at the B3LYP/6-31+G(d,p) level of theory.

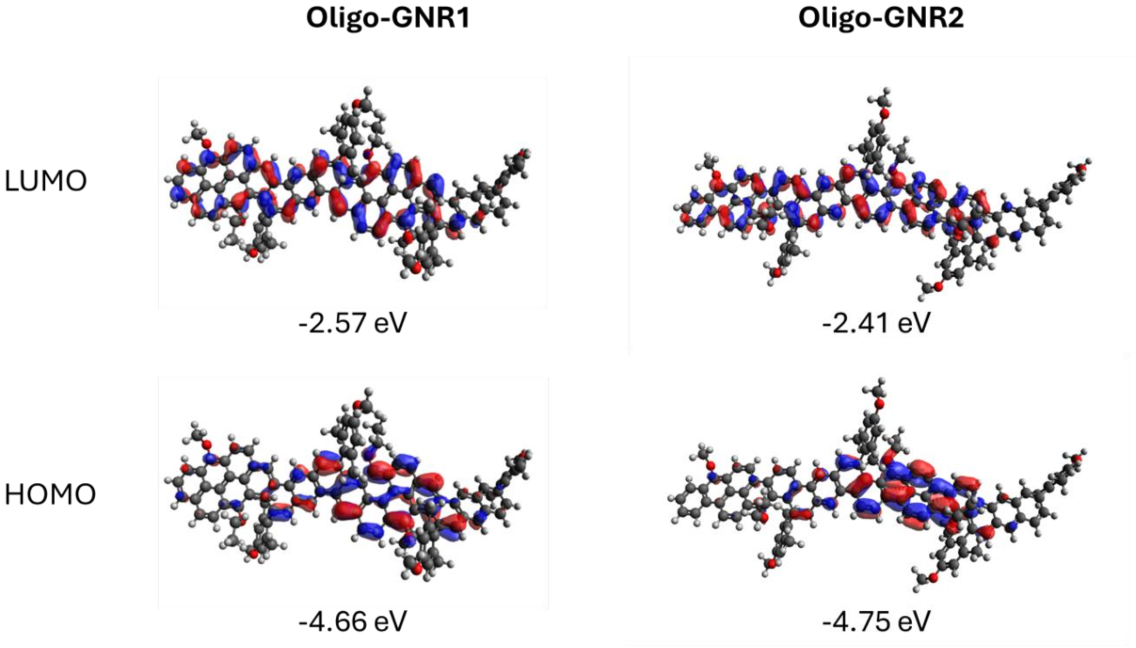
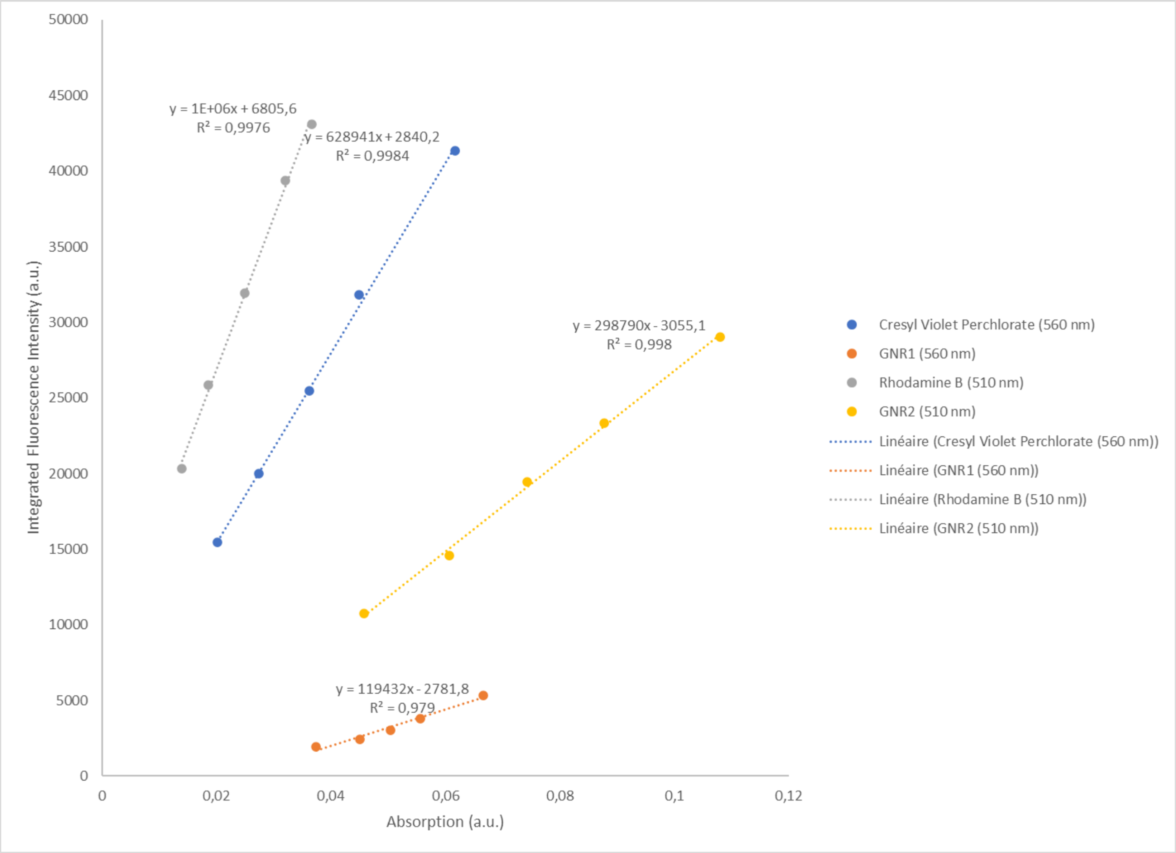


Figure S29. Kohn–Sham molecular orbitals of oligomers (two repeating units) of **GNR1** and **GNR2** based on calculations at the B3LYP/6-31+G(d,p) level of theory.

Fluorescence Quantum Yield

The quantum yields were determined using Cresyl Violet Perchlorate (ϕ_F = 0.54 in methanol) as the standard for **GNR1** and Rhodamine B (ϕ_F = 0.70 in ethanol) as the standard for **GNR2**. The calculations were performed using the following equation:

$$\boldsymbol{\Phi}_{F} = \boldsymbol{\Phi}_{ST}\ (\text{slope}_{GNR}/\text{slope}_{ST})(\boldsymbol{\eta}^2_{GNR}/\boldsymbol{\eta}^2_{ST})$$



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2 C. Aumaitre, D. Fong, A. Adronov and J.-F. Morin, *Polym. Chem.* **2019**, *10*, 6440.

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