Supplementary Information

Bis-Acenaphthoquinone Diimides with High Electron Deficiency and Good Coplanar Conformation

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Contents

1. Methods.

Bruker AVANCE 400 spectrometer was used to collect nuclear magnetic resonance spectra, including ^{1}H NMR and ^{13}C NMR spectra. MALDI-TOF mass spectra were recorded on a Bruker Biflex III MALDI-TOF Bruker instrument. Electrospray ionization (ESI) mass spectra were collected on an Orbitrap Fusion Lumos instrument. UV–vis absorption spectrum and PL spectrum were recorded in $CHCl_3$ solution by adopting a Perkin-Elmer Lamada 25 spectrophotometer and a Hitachi F-4600 spectrophotometer, respectively. The fluorescent quantum yields of BAIs in dichloromethane were measured by using an integrating sphere method on an Edinburgh FLS1000 instrument. For cyclic voltammetry measurement, a standard electrochemical workstation (CHI660E, Shanghai CHENHUA) with a three-electrode cell was used. This electrochemical cell contains a glassy carbon electrode, a Pt wire, and a Ag/AgCl (KCl, Sat'd) electrode, corresponding to the working electrode, counter electrode, and reference electrode, respectively. The CV curves of the samples were collected in an anhydrous and N_2-saturated dichloromethane solution in the presence of 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as the supporting electrolyte. Ferrocene (Fc) was used as the internal standard to calibrate the redox potential of the sample, and the onset oxidation of Fc/Fc^+ was determined as 0.38 V *vs* Ag/AgCl in our setup. Single-crystal X-ray data was collected on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer using graphite-monochromated Cu Kα radiation (λ = 1.54184 Å). Using Olex2, the structures were solved with the ShelXS structure solution program using Direct Methods and refined with the ShelXL refinement package using Least Squares minimization. The surface morphology of the annealed thin films was examined by using an atomic force microscope (AFM, Park XE7) in a tapping mode. The film microstructure was characterized by grazing incidence X-ray diffraction (GIXRD), and the relevant GIXRD data was collected at Shanghai Synchrotron Radiation Facility.

2. Transistor Devices Fabrication and Measurement.

Bottom-gate, top-contact transistors were fabricated on heavily *p*-doped Si wafers with a 300 nm thick SiO_2 layer. The substrates were first cleaned with piranha solution (volume mixing ratio: H_2SO_4: H_2O_2 = 2:1) for 20 min, then ultrasonically cleaned in deionized water and ethanol for 10 min each, and baked in oven at 70℃ for 20 min. After that, the substrates were modified by octadecyltrichlorosilane (OTS) in vapor phase in a vacuum oven at 120 ℃ for 3 h, followed by ultrasonic cleaning in hexane, ethanol, and chloroform for 5 min each. For BAI-1 and BAI-2 based transistors, the semiconducting layer was deposited on the OTS-treated substrates by spin-coating a chloroform solution (5 mg mL^{-1}) at a spin speed of 4000 rpm for 60 s, and then annealed in a vacuum oven at 120 ℃ for 30 min. The Ag source/drain electrodes were thermally evaporated onto the semiconducting layer through a shadow mask. The channel length and width of the transistor devices were 30 μm and 300 μm, respectively.

All the measurements were performed immediately in the nitrogen glovebox after the device fabrication was finished. The electrical characteristics were measured using a Keithley 4200A-SCS Parameter analyzer. The saturation mobility was calculated using the transistor equation:

$$I_d = \frac{WC_i\mu(V_g - V_{th})^2}{2L}$$

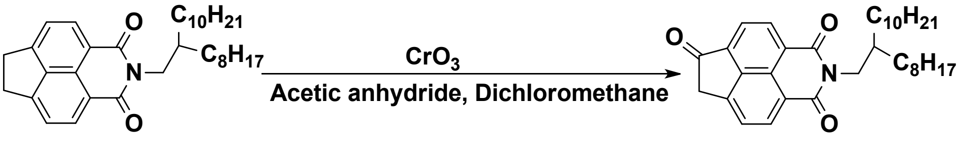
Where C_i (11.5 nF cm^{-2}) is the unit area capacitance of the SiO_2 dielectric; V_g and V_{th} represent the gate voltage and the threshold voltage, respectively.

3. Material Synthesis and Characterization.

All starting materials were obtained from commercial suppliers (e.g., Chem Greatwall and Derthon) and used as received. Solvents were dried and distilled according to standard procedures. For the contrast sample, *N*, *N′*-bis(2-ethylhexyl)naphthalene-1,4,5,8-tetracarboxylic acid diimide (NDI) was synthesized with reference to the literature.[1] Compound 1[2], compound 2[3], compound 3[2], compound 4[4], and diketone intermediates (9[2] and 10[4]), were synthesized according to the corresponding literature methods.

Synthesis of compound 5.

Compound 2 (500 mg, 0.99 mmol) was dissolved into a mixed solvent of dichloromethane (10 mL) and acetic anhydride (10 mL). CrO_3 (198 mg, 1.98 mmol) was then added to the solution by portions. The mixture was kept stirring at room temperature for 2 h. After that, the reaction mixture was quenched by ice water and then extracted with dichloromethane. The collected organic phase was dried with $MgSO_4$. After removal of the solvent, the crude material was further purified by column chromatography with petroleum ether: chloroform (2:1, v/v) as the eluent. Yield 353 mg (69 %) of a yellow-green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.67 (d, J = 7.2 Hz, 1H), 8.58 (d, J = 7.2 Hz, 1H), 8.13 (d, J = 7.2 Hz, 1H), 7.75 (d, J = 7.2 Hz, 1H), 4.13 (d, J = 7.2 Hz, 2H), 3.99 (s, 2H), 2.03 – 1.92 (br, 1H), 1.32 – 1.21 (m, 32H), 0.86 (dd, J = 14, 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.08, 164.03, 163.74, 141.70, 141.21, 138.11, 132.88, 131.91, 125.95, 125.86, 122.46, 122.24, 120.57, 53.54, 44.72, 42.64, 36.66, 31.92, 31.89, 31.71, 31.68, 30.04, 30.02, 29.64, 29.61, 29.57, 29.34, 29.30, 26.51, 26.49, 22.69, 22.67, 14.12, 14.05. HRMS: m/z $[M+H]^+$ calcd for ($C_{34}H_{48}NO_3$): 518.3628; found 518.3630.



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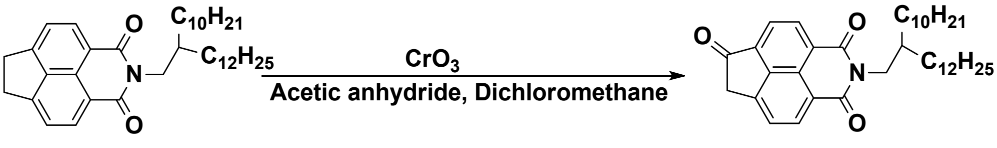
Synthesis of compound 6.

Compound 3 (500 mg, 0.89 mmol) was dissolved into a mixed solvent of dichloromethane (10 mL) and acetic anhydride (10 mL). CrO_3 (178 mg, 1.78 mmol) was then added to the solution by portions. The mixture was kept stirring at room temperature for 2 h. After that, the reaction mixture was quenched by ice water and then extracted with dichloromethane. The collected organic phase was dried with $MgSO_4$. After removal of the solvent, the crude material was further purified by column chromatography with petroleum ether: chloroform (2:1, v/v) as the eluent. Yield 331 mg (65 %) of a yellow-green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.68 (d, J = 7.2 Hz, 1H), 8.59 (d, J = 7.2 Hz, 1H), 8.14 (d, J = 7.2 Hz, 1H), 7.75 (d, J = 7.2 Hz, 1H), 4.13 (d, J = 7.2 Hz, 2H), 3.99 (s, 2H), 1.98 (br, 1H), 1.41 – 1.09 (m, 30H), 0.86 (td, J = 6.8, 2.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.11, 164.05, 163.76, 141.69, 141.22, 138.12, 132.89, 131.93, 125.97, 125.87, 122.46, 122.25, 120.58, 44.73, 42.64, 36.67, 31.93, 31.71, 30.04, 29.68, 29.66, 29.64, 29.62, 29.37, 29.34, 26.51, 22.70, 14.13. HRMS: m/z $[M+H]^+$ calcd for ($C_{38}H_{55}NO_3$): 574.4255; found: 574.4249.



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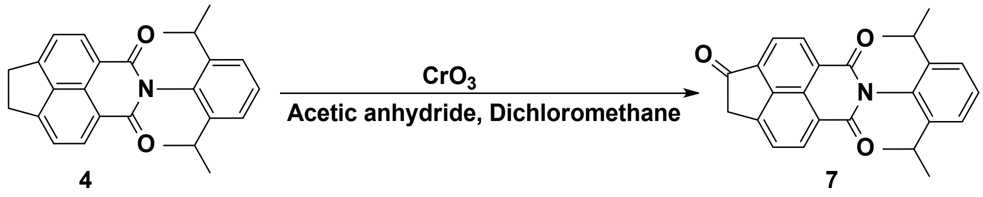
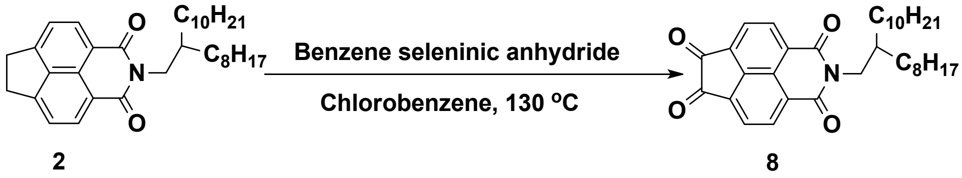
Synthesis of compound 7.

Compound **4** (500 mg, 1.30 mmol) was dissolved into a mixed solvent of dichloromethane (10 mL) and acetic anhydride (10 mL). CrO_3 (260 mg, 260 mmol) was then added to the solution by portions. The mixture was kept stirring at room temperature for 2 h. After that, the reaction mixture was quenched by ice water and then extracted with dichloromethane. The collected organic phase was dried with $MgSO_4$. After removal of the solvent, the crude material was further purified by column chromatography with petroleum ether: chloroform (2:1, v/v) as the eluent. Yield 352 mg (68 %) of a yellow-green solid. ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.76 (d, J = 7.2 Hz, 1H), 8.67 (d, J = 7.2 Hz, 1H), 8.20 (d, J = 7.2 Hz, 1H), 7.82 (d, J = 7.2 Hz,1H), 7.49 (t, J = 7.8 Hz, 1H), 7.34 (d, J = 7.6 Hz, 2H), 4.05 (d, J = 1.2 Hz, 2H), 2.73 (m, 2H), 1.16 (dd, J = 6.8, 2.4 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 200.12, 163.73, 163.47, 145.64, 142.19, 141.40, 138.48, 133.46, 132.50, 130.70, 129.65, 126.67, 125.78, 124.11, 122.58, 122.35, 120.48, 42.65, 29.13, 23.98. HRMS: m/z $[M+H]^+$ calcd for ($C_{26}H_{23}NO_3$): 398.1751; found: 398.1759.



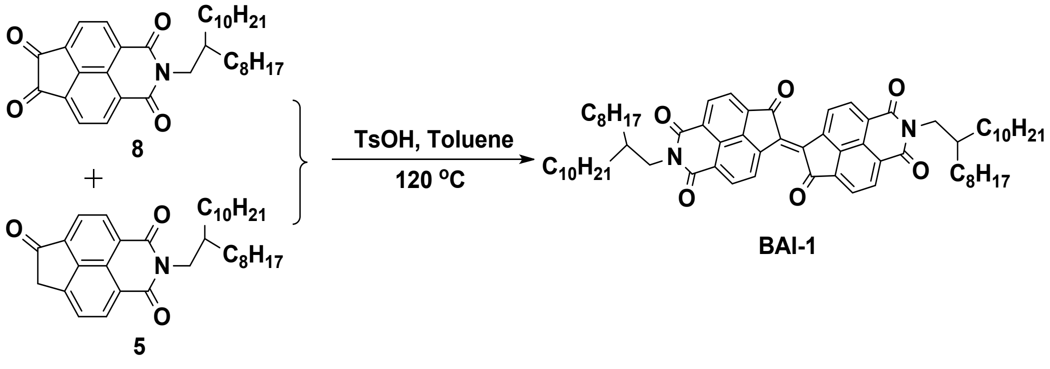
Synthesis of compound 8.

Compound 8 was prepared by CrO_3-oxidation method reported by Pei group [2], while the structural characterization of compound 8 was not confirmed. To address this issue, herein we reported an improved method and characterized its chemical structure. To a mixture solution of compound 2 (1.0 g, 1.99 mmol) and 15 mL of chlorobenzene, BSA (2.15 g, 5.97 mmol) was added. The mixture was then stirred at 130 °C for 36 h. After cooling down to the room temperature, the organic phase was obtained by dichloromethane extraction and then dried with $MgSO_4$. After removal of the solvent, the crude product was further purified by column chromatography with petroleum ether: chloroform (2:1, v/v) as the eluent. Yield 824 mg (78 %) of a yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.81 (d, J = 7.2 Hz, 2H), 8.36 (d, J = 7.2 Hz, 2H), 4.17 (d, J = 7.2 Hz, 2H), 1.32 (br, 1H), 1.38 – 1.22 (m, 32H), 0.86 (q, J = 12.8, 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 186.26, 162.91, 143.82, 132.17, 131.99, 126.75, 126.26, 122.94, 45.14, 36.65, 31.92, 31.88, 31.66, 30.02, 29.63, 29.61, 29.56, 29.34, 29.29, 26.44, 22.69, 22.66, 14.12. HRMS: m/z $[M+H]^+$ calcd for ($C_{34}H_{46}NO_4$): 532.3421; found 532.3426.



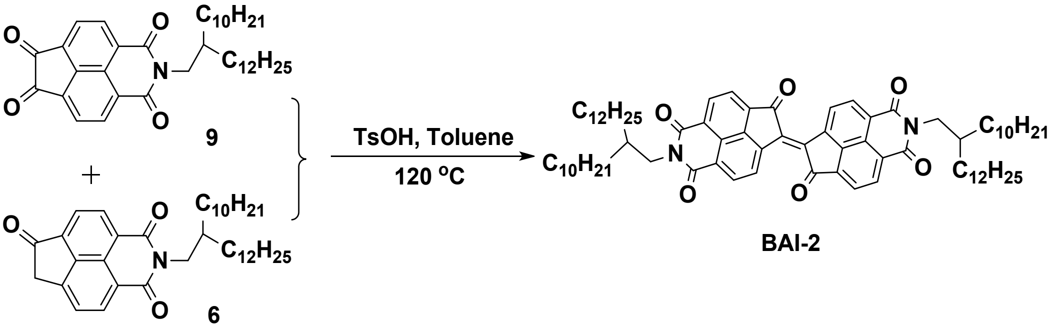
Synthesis of compound BAI-1.

Under nitrogen atmosphere, a mixture solution of compound 4 (100 mg, 0.19 mmol), compound 6 (103 mg, 0.19 mmol), TsOH (9 mg, 0.05 mmol), and 10 mL of toluene was refluxed for 12 h. After that, the organic phase was collected by dichloromethane extraction and then dried with $MgSO_4$. After removal of the solvent under reduced pressure, the residue was further purified by column chromatography with petroleum ether: chloroform (1:1, v/v). Yield 127 mg (65%) of an orange-yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.56 (d, J = 8.0 Hz, 2H), 8.65 (dd, J = 7.2, 2.0 Hz, 4H), 8.20 (d, J = 7.2 Hz, 2H), 4.14 (d, J = 7.6 Hz, 4H), 2.00 (s, 2H), 1.55 – 1.08 (m, 64H), 0.85 (td, J = 6.8, 2.4 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.10, 163.07, 162.94, 139.48, 138.87, 136.70, 134.41, 132.69, 131.18, 129.24, 125.89, 125.09, 122.99, 122.29, 44.80, 36.72, 31.92, 31.89, 31.69, 30.07, 29.67, 29.64, 29.60, 29.35, 29.33, 26.49, 22.67, 14.11. HRMS: m/z $[M+H]^+$ calcd for ($C_{68}H_{91}N_2O_6$): 1031.6871; found 1031.6879.



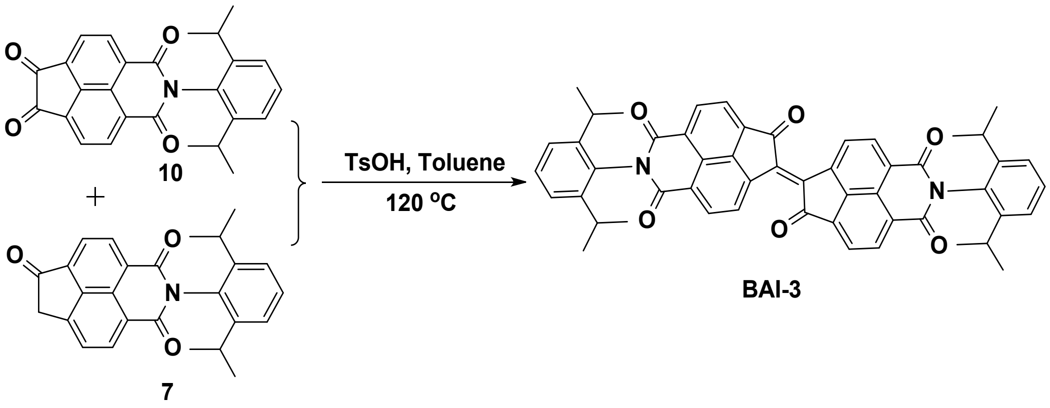
Synthesis of compound BAI-2.

Under nitrogen atmosphere, a mixture solution of compound 4 (100 mg, 0.17 mmol), compound 6 (102 mg, 0.17 mmol), TsOH (9 mg, 0.05 mmol), and toluene (10 mL) was refluxed for 12 h. After cooling down to the room temperature, the reaction mixture was extracted with dichloromethane and dried with $MgSO_4$. After that, the solvent was removed under reduced pressure. The residue was purified by column chromatography with petroleum ether: chloroform (1:1, v/v). Yield 140 mg (70%) of an orange-yellow solid. ^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm) 9.66 (d, J = 8.0 Hz, 2H), 8.74 (dd, J = 8.0, 4.0 Hz, 4H), 8.29 (d, J = 7.2 Hz, 2H), 4.16 (d, J = 7.2 Hz, 4H), 2.00 (br, 2H), 1.44 – 1.10 (m, 80H), 0.86 (t, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, CDCl$_3$) δ (ppm) 192.17, 163.14, 162.80, 139.73, , 139.14, 136.96, 134.47, 132.75, 131.24, 129.28, 126.03, 125.30, 123.11, 122.34, 44.86, 36.74, 31.94, 31.74, 30.08, 29.72, 29.69, 29.66, 29.38, 26.52, 22.70, 14.12. HRMS: m/z [M+H]$^+$ calcd for ($C_{76}H_{107}N_2O_6$): 1143.8123; found 1143.8129.



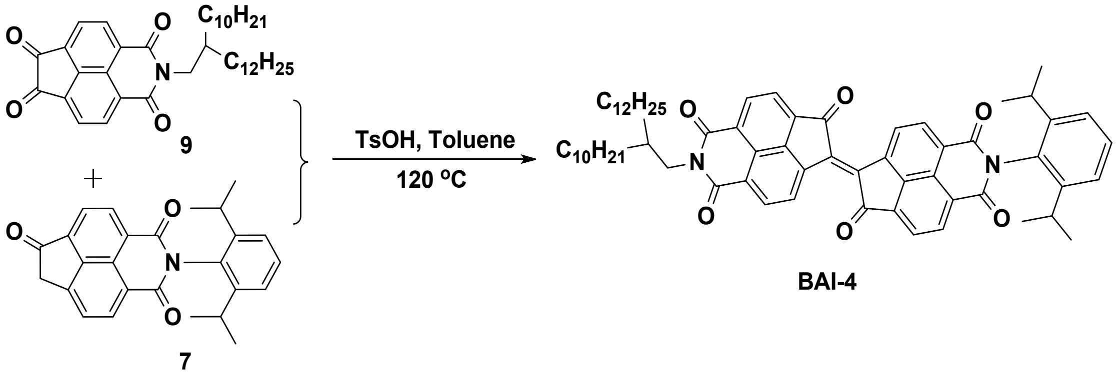
Synthesis of compound BAI-3.

Under nitrogen atmosphere, a mixture solution of compound 5 (100 mg, 0.25 mmol), compound 7 (103 mg, 0.25 mmol), TsOH (9 mg, 0.05 mmol), and toluene (10 mL) was refluxed for 12 h. After cooling down to the room temperature, the reaction mixture was extracted with dichloromethane and dried with MgSO$_4$, followed by removing solvent under reduced pressure. The residue was purified by column chromatography with petroleum ether: chloroform (1:1, v/v). Yield 143 mg (72%) of an orange-yellow solid. ^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm) 9.76 (d, J = 8.0 Hz, 2H), 8.86 – 8.82 (dd, J = 10.8, 8.0 Hz, 4H), 8.36 (d, J = 7.2 Hz, 2H), 7.51 (d, J = 7.6 Hz, 2H), 7.36 (d, J = 8.0 Hz, 4H), 2.80 – 2.74 (m, 4H), 1.19 (dd, J = 7.2, 4.4 Hz, 24H). ^{13}C NMR (100 MHz, CDCl$_3$) δ (ppm) 192.59, 163.34, 163.16, 145.64, 140.35, 139.64, 137.75, 135.45, 133.59, 132.16, 130.49, 129.82, 129.45, 126.36, 126.15, 124.21, 123.22, 122.65, 29.23, 24.03. HRMS: m/z [M+H]$^+$ calcd for ($C_{52}H_{42}N_2O_6$): 791.3116; found 791.3114.



Synthesis of compound BAI-4.

Under nitrogen atmosphere, a mixture solution of compound 7 (150 mg, 0.38 mmol), compound 9 (221 mg, 0.38 mmol), TsOH (9 mg, 0.05 mmol), and toluene (10 mL) was refluxed for 12 h. After cooling down to the room temperature, the organic phase was collected by dichloromethane extraction and then dried with $MgSO_4$. After removal of solvent under reduced pressure, the residue was purified by column chromatography with petroleum ether: chloroform (1:1, v/v). Yield 248 mg (68%) of an orange-yellow solid. ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.71 (dd, J = 8, 4.8 Hz, 2H), 8.86 – 8.72 (m, 4H), 8.32 (dd, J = 15.6, 7.2 Hz, 2H), 7.50 (t, J = 7.6 Hz, 1H), 7.35 (d, J = 7.6 Hz, 2H), 4.18 (d, J = 7.2 Hz, 2H), 2.77 (m, 2H), 1.93 (br, 1H), 1.45 – 1.14 (m, 52H), 0.86 (t, J = 6.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.41, 192.04, 163.35, 163.27, 163.21, 163.09, 145.66, 140.13, 139.93, 139.50, 139.17, 137.53, 137.13, 135.22, 134.84, 133.46, 132.97, 131.99, 131.45, 130.49, 129.80, 129.37, 126.26, 126.19, 126.05, 125.43, 124.19, 123.21, 122.48, 44.85, 36.67, 31.92, 31.70, 30.04, 29.69, 29.67, 29.65, 29.64, 29.62, 29.37, 29.35, 29.21, 26.49, 24.06, 22.69, 14.12. HRMS: m/z $[M+H]^+$ calcd for ($C_{64}H_{74}N_2O_6$): 967.5620; found 967.5617.



4. X-Ray Crystallographic Analysis.

Table S1. Crystal data and structure refinement of BAI-3.

Empirical formula	$C_{52}H_{42}N_2O_6$
Formula weight	790.87
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	16.1033(9)
b/Å	8.4274(5)
c/Å	34.064(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4622.8(6)
Z	4
ρ_{calc}g/cm^3	1.136
μ/mm^{-1}	0.595
F(000)	1664.0
Crystal size/mm^3	0.11 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.188 to 147.628
Index ranges	$-19 \leq h \leq 19$, $-10 \leq k \leq 5$, $-38 \leq l \leq 41$
Reflections collected	11837
Independent reflections	6790 [R_{int} = 0.0581, R_{sigma} = 0.0739]
Data/restraints/parameters	6790/33/550
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0859, wR_2 = 0.2261
Final R indexes [all data]	R_1 = 0.0986, wR_2 = 0.2443
Largest diff. peak/hole / e Å^{-3}	0.47/-0.55
Flack parameter	0.1(6)
CCDC number	2085221

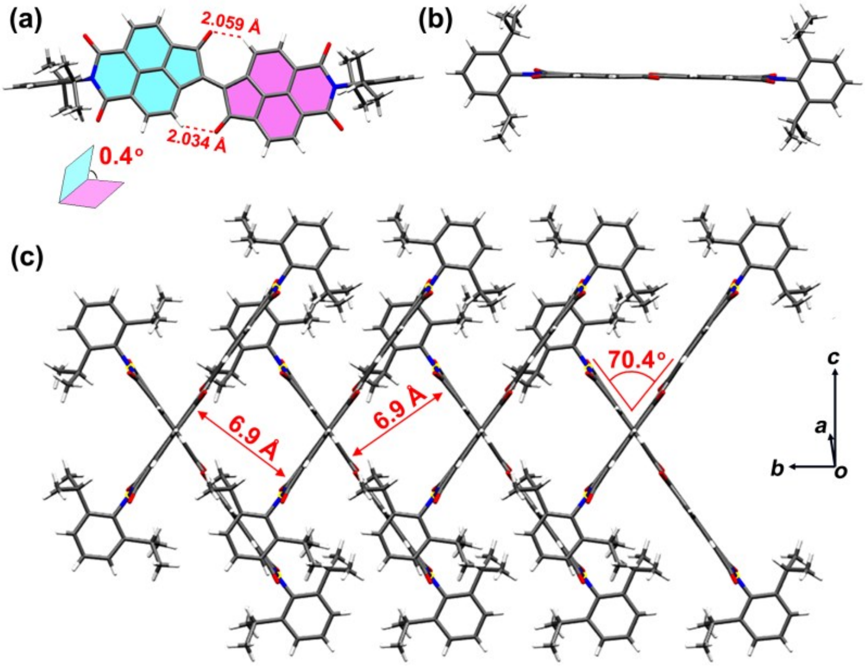


Figure S1. Crystal structure of BAI-3. (a) Top view and (b) side view of BAI-3 crystal. (c) Crystal packing structure.

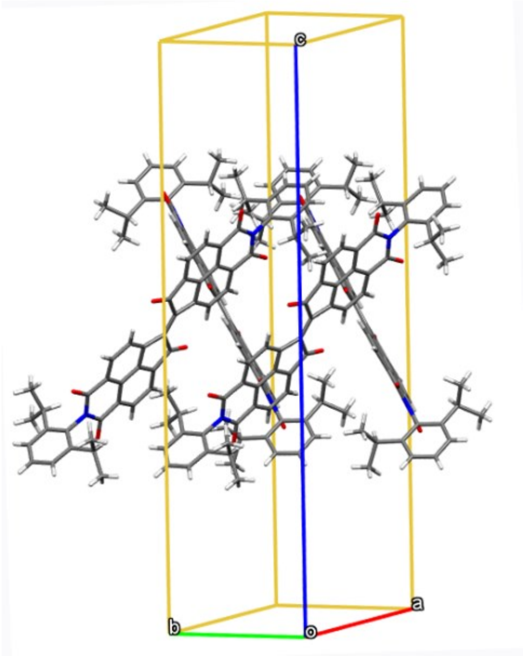


Figure S2. Crystal packing structure of BAI-3.

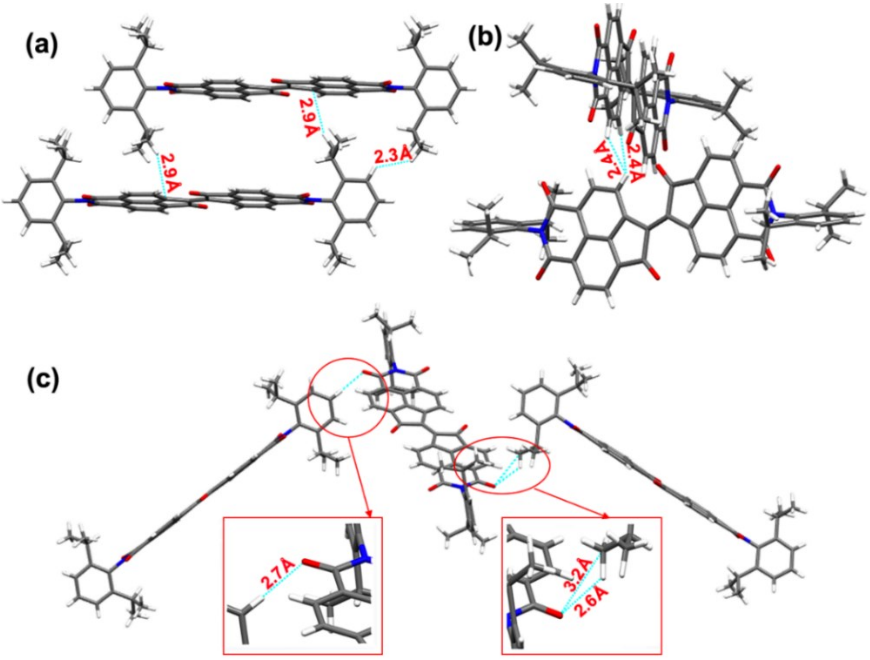


Figure S3. Crystal organization of BAI-3 involves multiple weak intermolecular interactions, including C–H···C (2.9 Å), C–H···C–H (2.3 and 2.4 Å), C···O (3.2 Å), and C–H···O (2.6 and 2.7 Å) interactions.

5. Opto-electrical Properties.

Table S2. Summary of opto-electrical properties of BAIs and their analogue NDI.

Compd	$^a\lambda_{max}$ (nm)/ε ($\times 10^4 \cdot M^{-1} \cdot cm^{-1}$)	$^a\lambda_{onset}$ (nm)	$^bE_g^{opt}$ (eV)	$^a\lambda_{em}$ (nm)	Φ_F^{sol} (%)	E_{red} (V)	$^cE_{LUMO}$ (eV)	$^dE_{HOMO}$ (eV)	$^eE_{LUMO}$ (eV)	$^eE_{HOMO}$ (eV)
BAI-1	322/3.7, 410/2.7	550	2.25	579	2.0	–0.34	-4.08	–6.33	–3.55	–6.56
BAI-2	322/3.8, 409/2.8	550	2.25	579	1.9	–0.34	–4.08	–6.33	–3.55	–6.56
BAI-3	322/5.8, 411/4.4	550	2.25	581	2.7	–0.33	–4.09	–6.34	–3.56	–6.49
BAI-4	322/4.6, 410/3.4	550	2.25	580	1.9	–0.32	–4.10	–6.35	–3.56	–6.49
NDI	360/2.2, 380/2.7	390	3.17	416	0.1	–0.57	–3.85	–7.02	–3.40	–7.03

[a]Measured in $CHCl_3$ solution (1.0×10^{-5} M). [b]$E_g^{opt} = 1240/\lambda_{onset}$. [c]$E_{LUMO} = -(E_{red} + 4.42)$ eV. [d]$E_{HOMO} = (E_{LUMO} - E_g^{opt})$ eV. [e]Calculated by DFT at the B3LYP/6-31G(d) level.

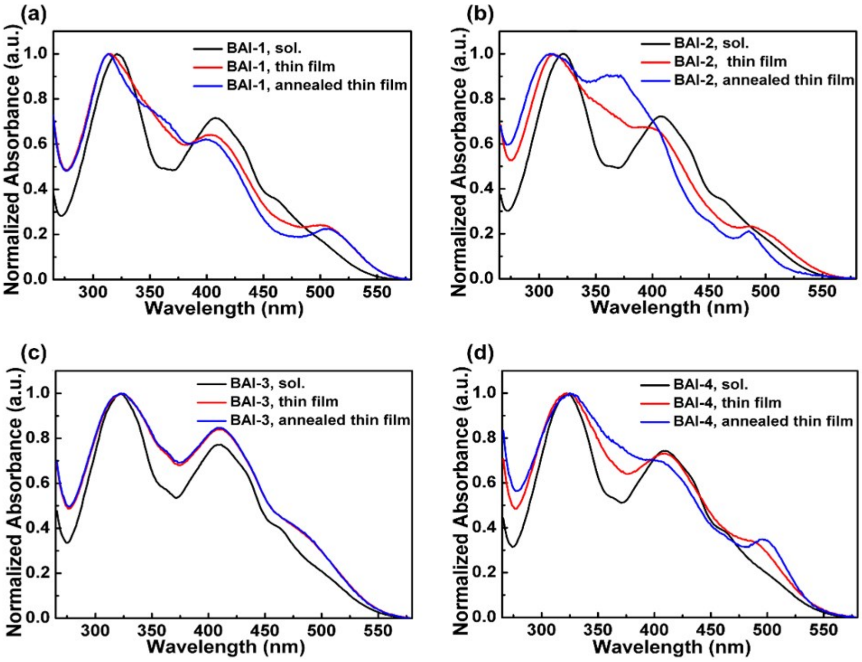


Figure S4. Absorption spectra of BAI-1(a), BAI-2 (b), BAI-3 (c), and BAI-4 (d) in chloroform solution and thin films with/without annealing treatment at 120 °C for 10 min.

6. DFT Theoretical Calculation.

Density functional theory (DFT) calculations have been performed at the B3LYP/6-31G(d) level of theory, as implemented in the Gaussian 09 program package. [5] The UV-Vis absorption spectra were calculated using time-dependent density functional theory (TD-DFT) linear response method at PBE0/Def2TZVP level of theory.[6] The solvent effect of $CHCl_3$ was taken into account by a polarizable continuum model.[7] In order to reduce computational time, the alkyl side chains were substituted by methyl groups in the DFT calculations.

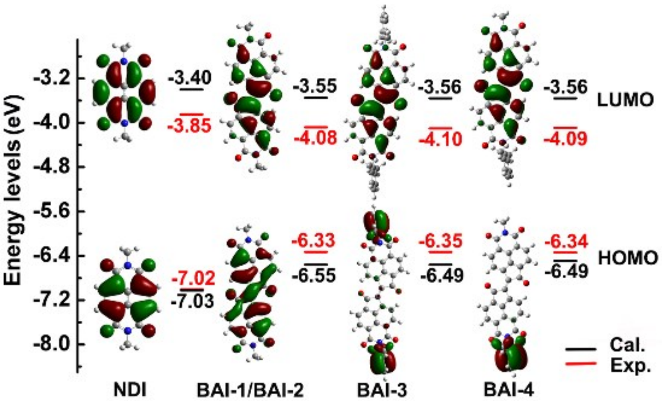


Figure S5. Optimized molecular orbital profiles and the energy diagrams of the HOMOs and LUMOs obtained from experiment and calculation.

Table S3. Theoretical simulation spectral data of BAI-1.

Compd	Excited States	Energy (eV)	Wavelength (nm)	Osc. Strength	Main contributions
BAI-1	1	2.5707 eV	482.30 nm	0.33940	HOMO→LUMO 81.0% HOMO-2→LUMO 12.4%
	2	2.8387 eV	436.76 nm	0.24540	HOMO-2→LUMO 56.8% HOMO→LUMO 17.4% HOMO-2→LUMO+1 5.9% HOMO→LUMO+1 5.2%
	4	2.9861 eV	415.20 nm	0.26910	HOMO→LUMO+1 90.8% HOMO-2→LUMO 5.7%
	9	3.5225 eV	351.98 nm	0.22530	HOMO-2→LUMO+1 36.9% HOMO-1→LUMO+2 32.6% HOMO-4→LUMO 6.6% HOMO-5→LUMO+2 5.2% HOMO-2→LUMO 5.1%
	10	3.5551 eV	348.75 nm	0.26970	HOMO-1→LUMO+2 52.6% HOMO-2→LUMO+1 15.5% HOMO-4→LUMO 10.8% HOMO-1→LUMO+1 8.3%
	17	3.8776 eV	319.74 nm	0.61190	HOMO-6→LUMO 41.3% HOMO-7→LUMO 32.6% HOMO-10 →LUMO 9.2%
	21	4.1015 eV	302.29 nm	0.16700	HOMO-7 → LUMO +1 34.5% HOMO-10 → LUMO 25.9% HOMO-8 → LUMO +2 11.4% HOMO-6 → LUMO +1 10.8%

7. Output curves of BAI-1 and BAI-2 Transistors.

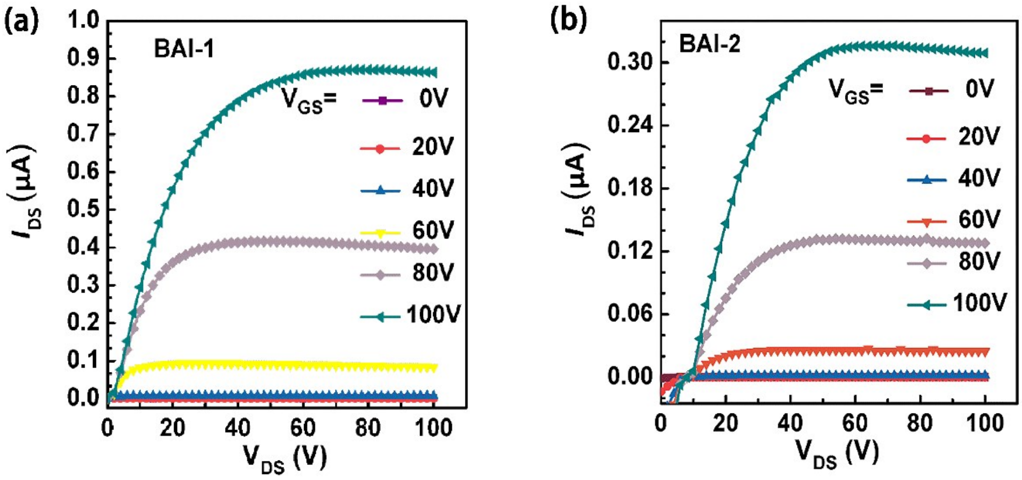


Figure S6. Typical output curves of BAI-1 (a) and BAI-2 (b) based transistors.

8. Mobility Statistics from 30 Transistor Devices.

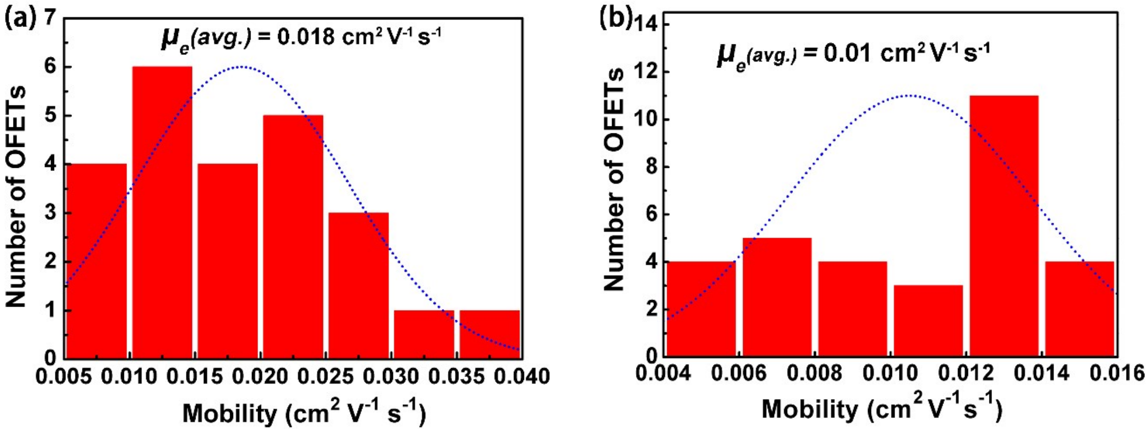


Figure S7. Mobility statistics of 30 OFET devices fabricated from BAI-1 (a) and BAI-2 (b) annealed thin films.

9. GIXRD Data of BAI-1 and BAI-2 Thin Films.

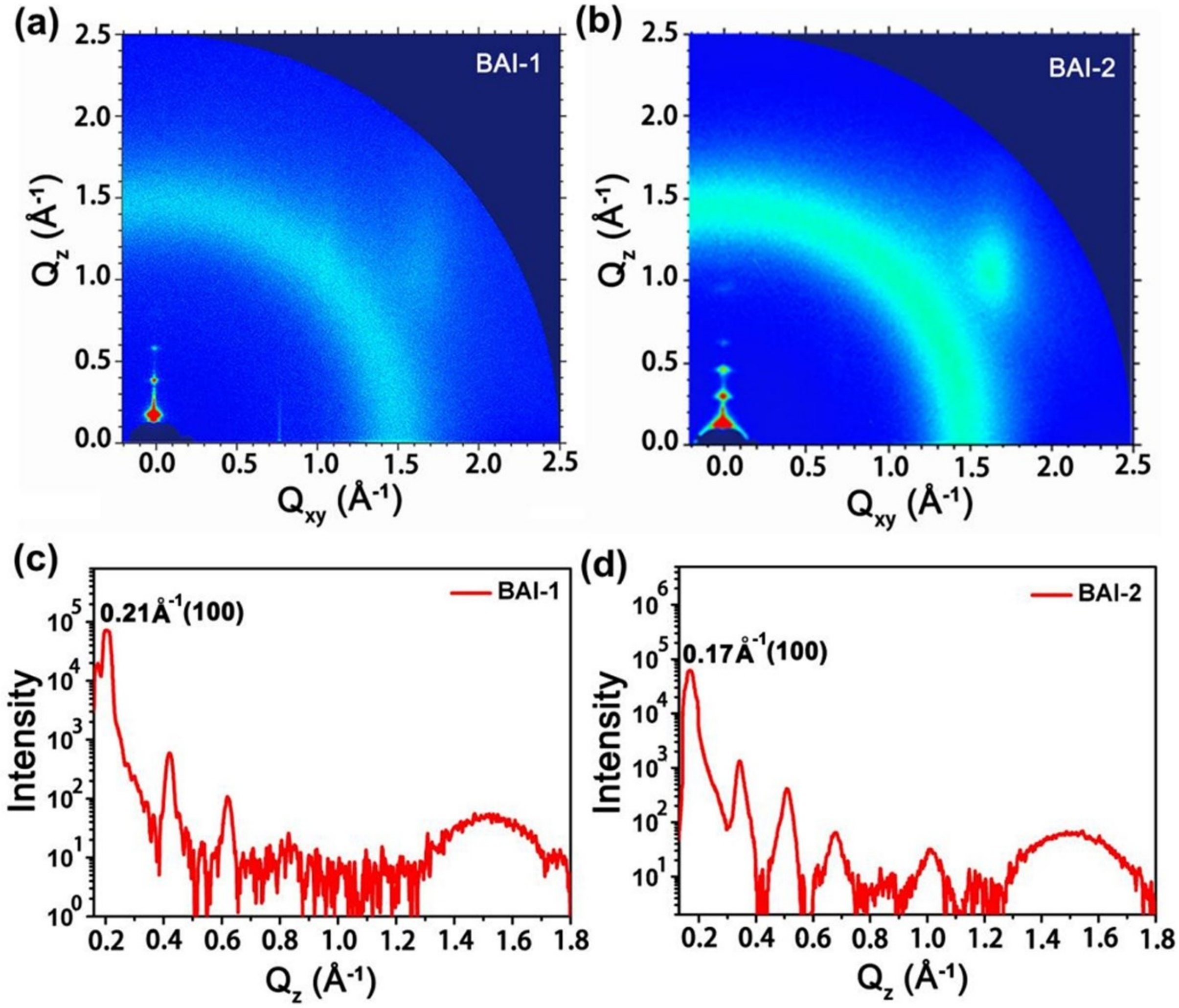


Figure S8. GIXRD data of the BAI-1 and BAI-2 annealed thin films deposited on the OTS-modified SiO_2/Si substrates, (a and b) 2D-GIXRD pattern, (c and d) Corresponding GIXRD line cuts along the out-of-plane (Qz) direction.

10. ^{1}H NMR and ^{13}C NMR Spectra

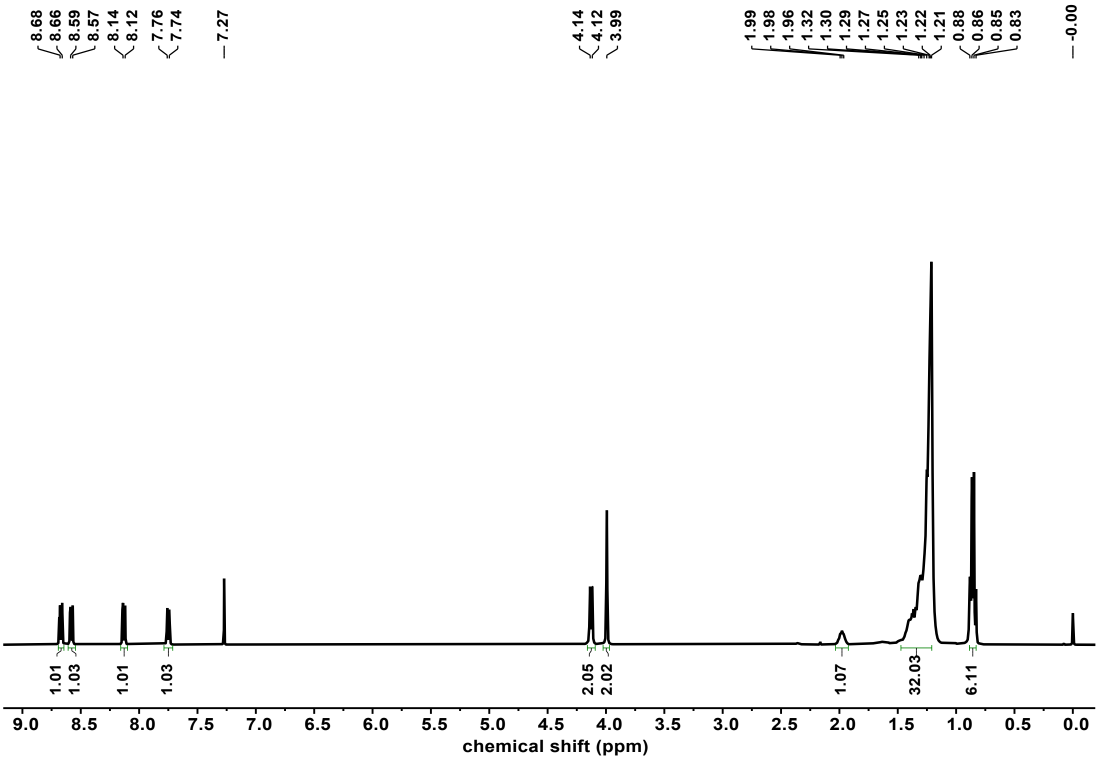


Figure S9. ^{1}H NMR spectrum of compound 5 ($CDCl_3$, 25 °C).

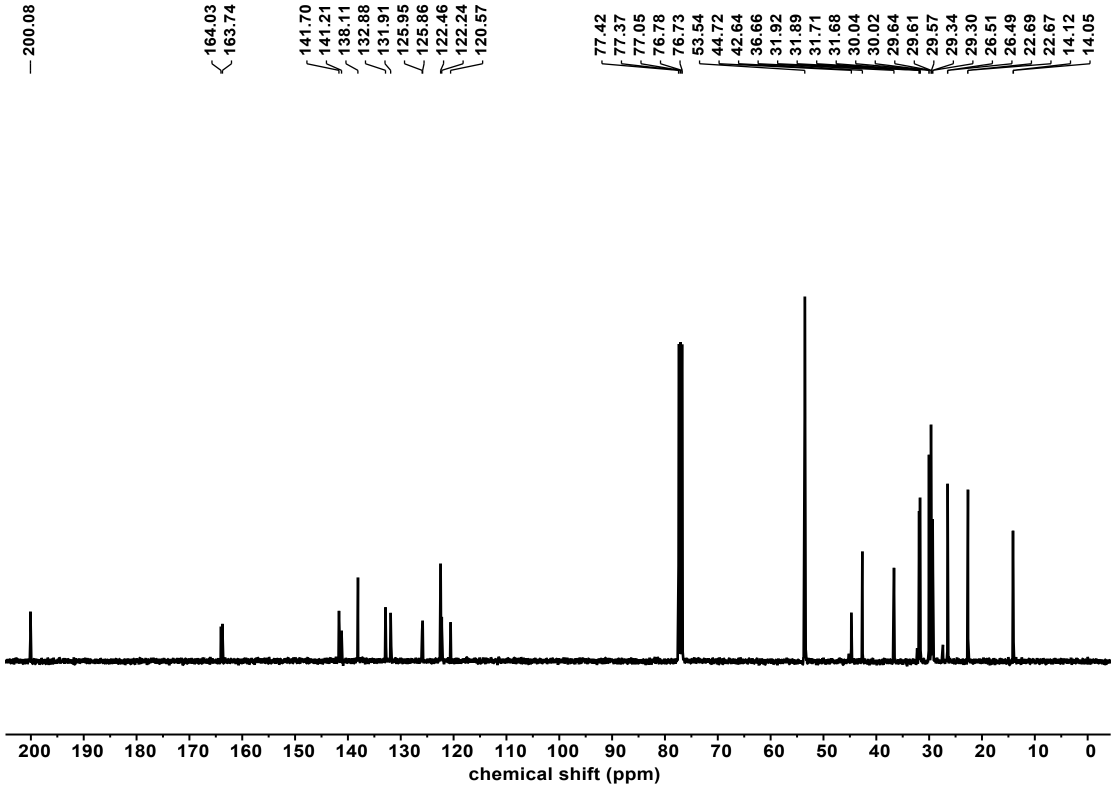


Figure S10. ^{13}C NMR spectrum of compound 5 ($CDCl_3$, 25 °C).

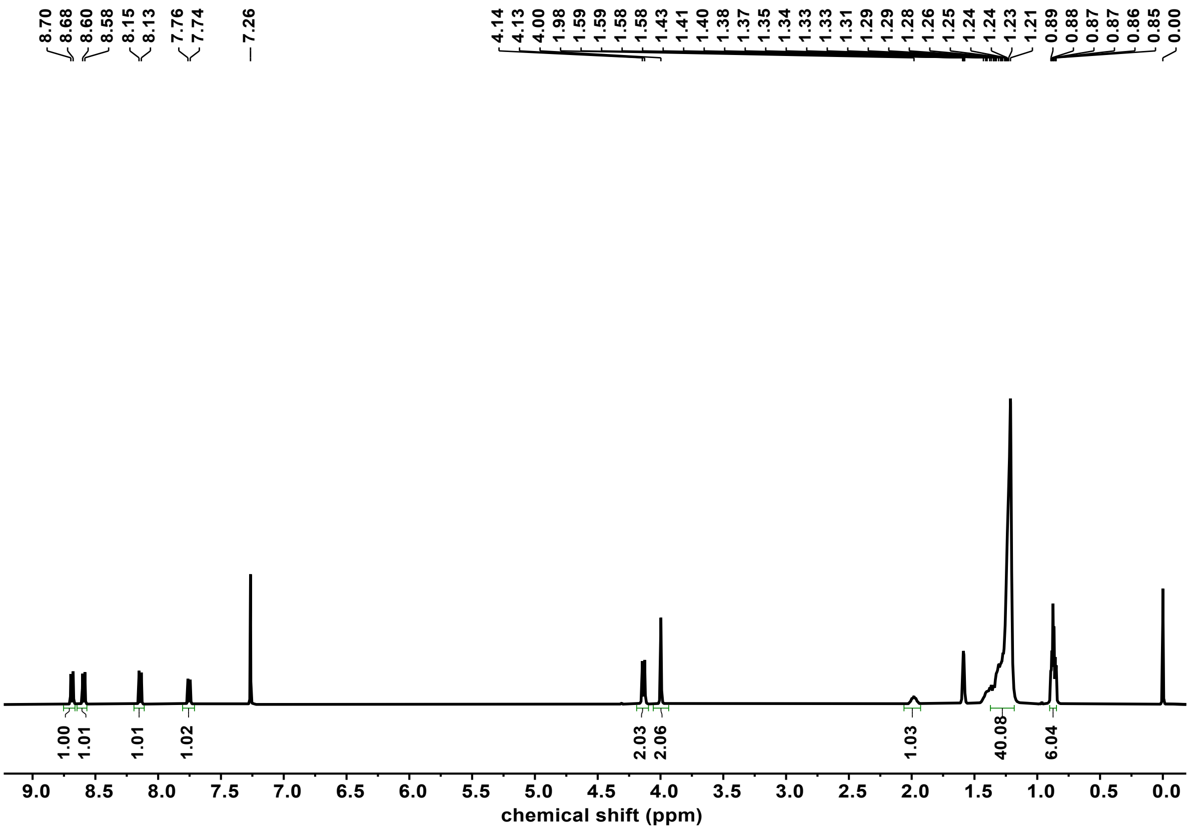


Figure S11. ^{1}H NMR spectrum of compound 6 ($CDCl_3$, 25 ^oC).

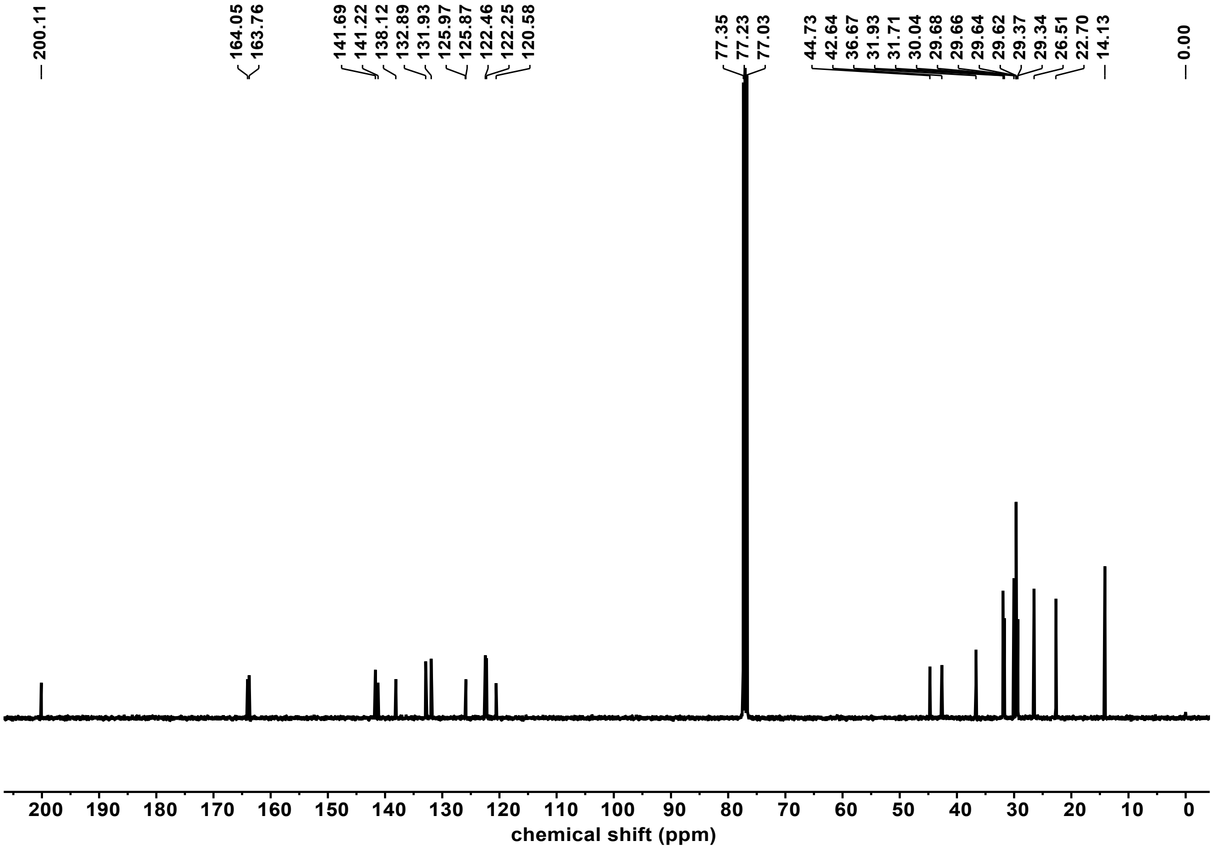


Figure S12. ^{13}C NMR spectrum of compound 6 ($CDCl_3$, 25 ^oC).

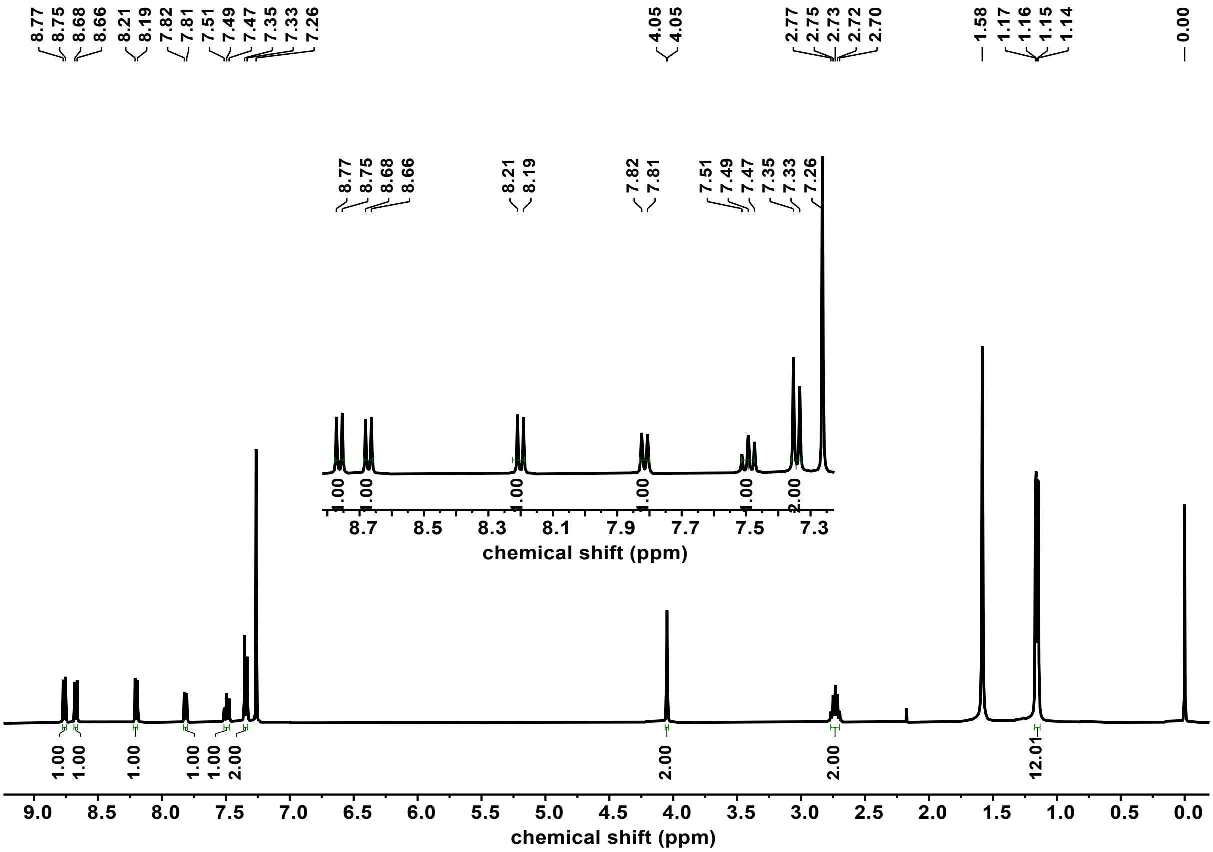


Figure S13. ^{1}H NMR spectrum of compound 7 ($CDCl_3$, 25 °C).

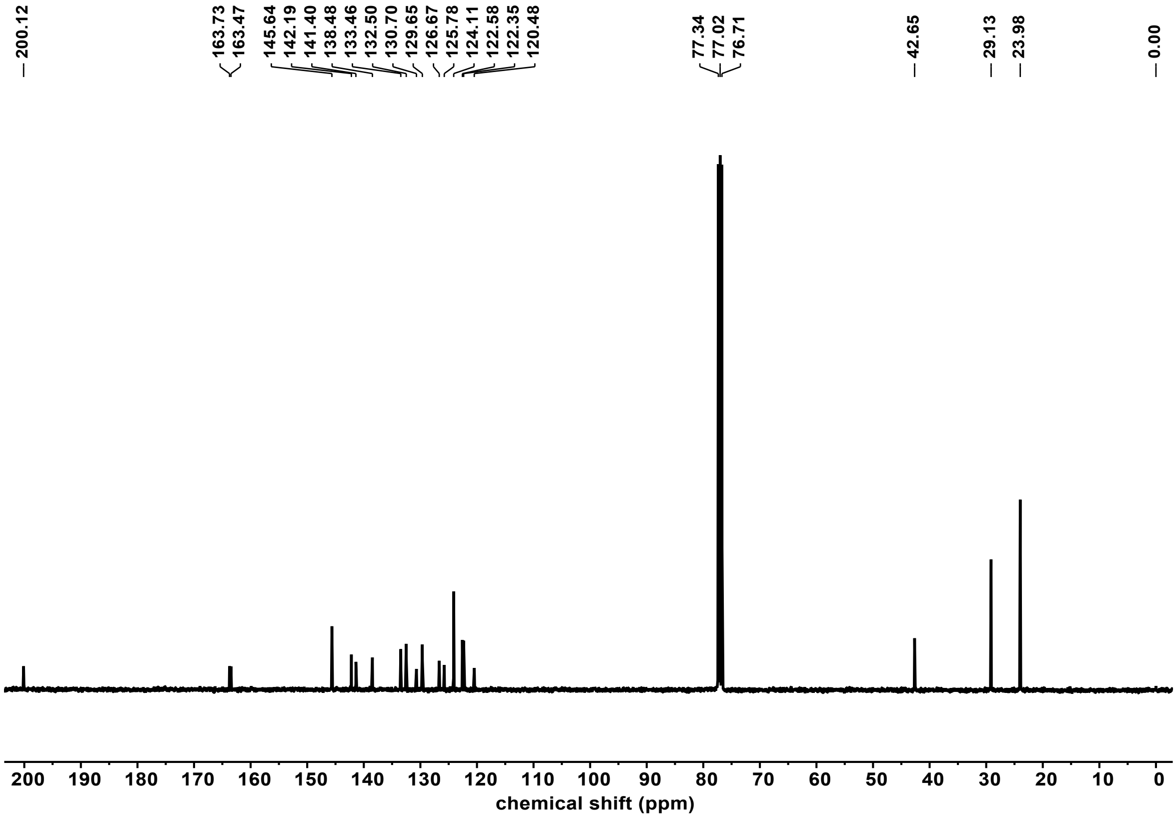


Figure S14. ^{13}C NMR spectrum of compound 7 ($CDCl_3$, 25 °C).

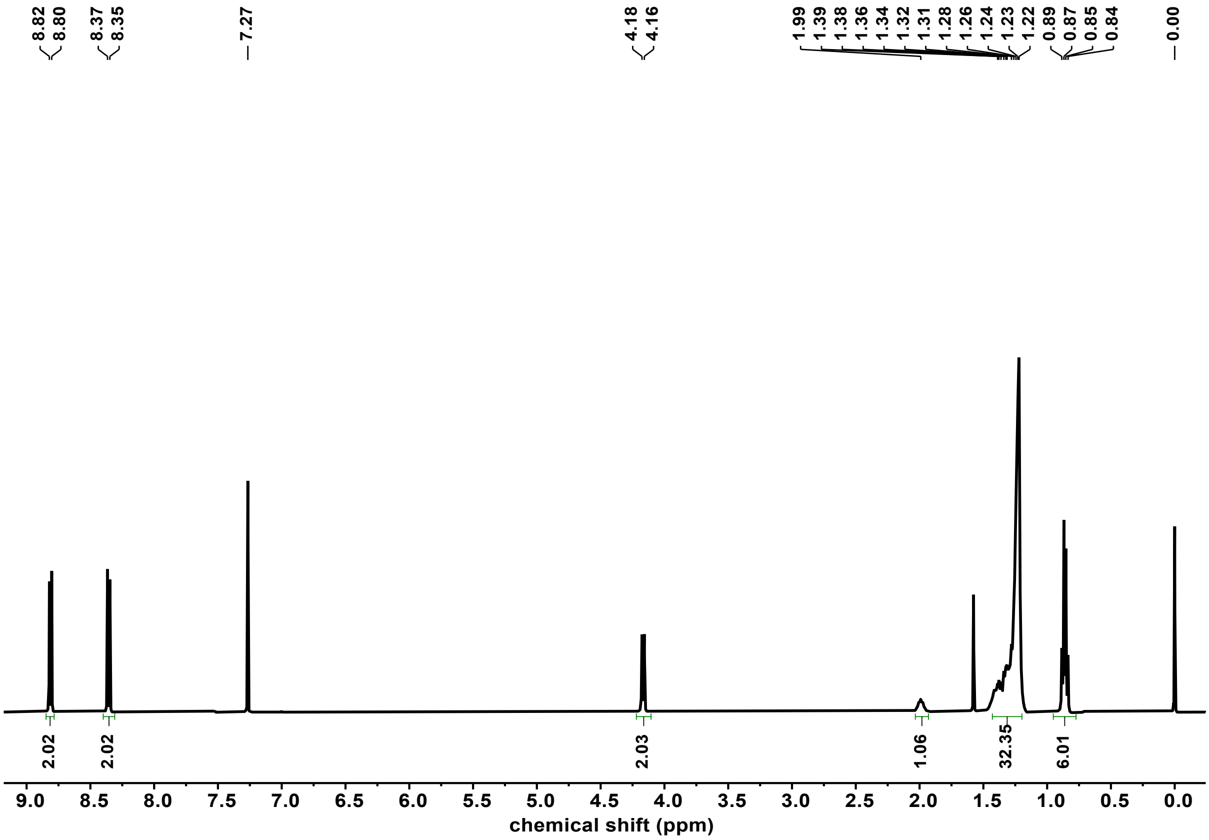


Figure S15. ^{1}H NMR spectrum of compound 8 (CDCl$_3$, 25 ^{o}C).

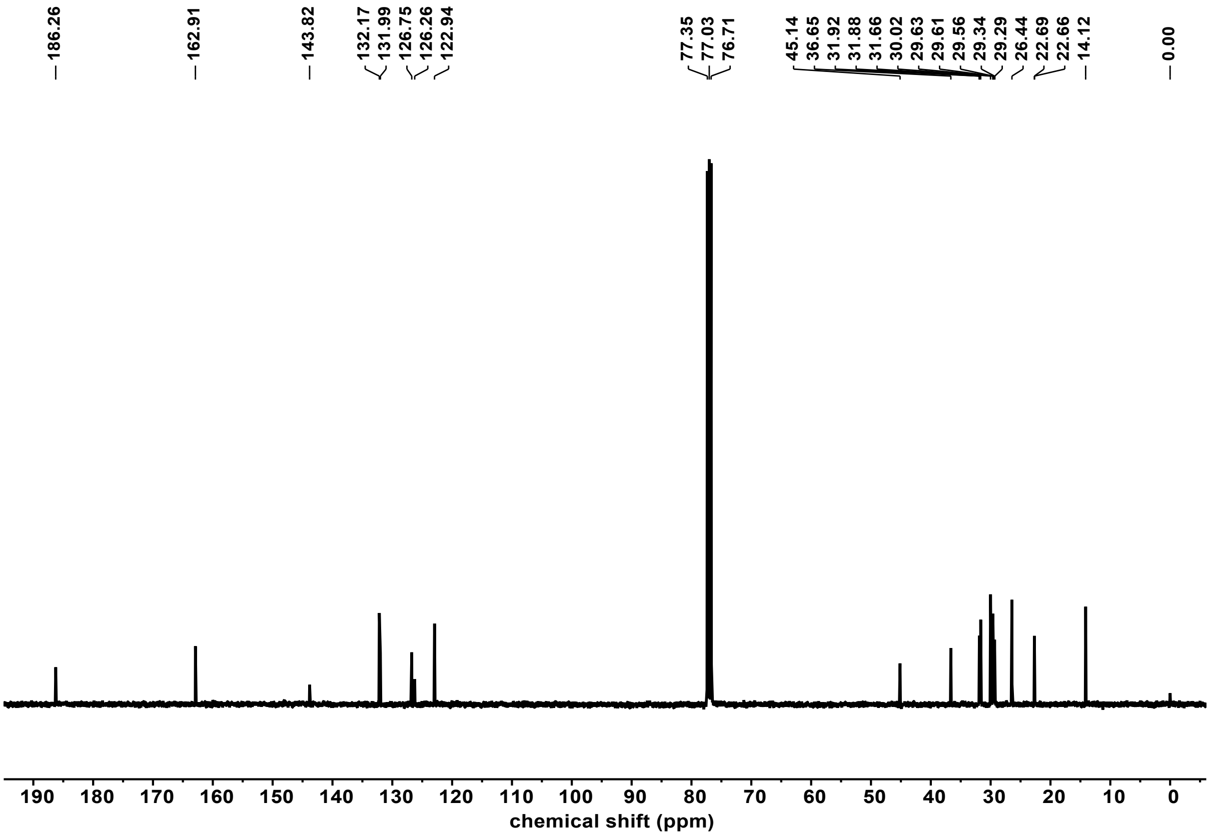


Figure S16. ^{13}C NMR spectrum of compound 8 (CDCl$_3$, 25 ^{o}C).

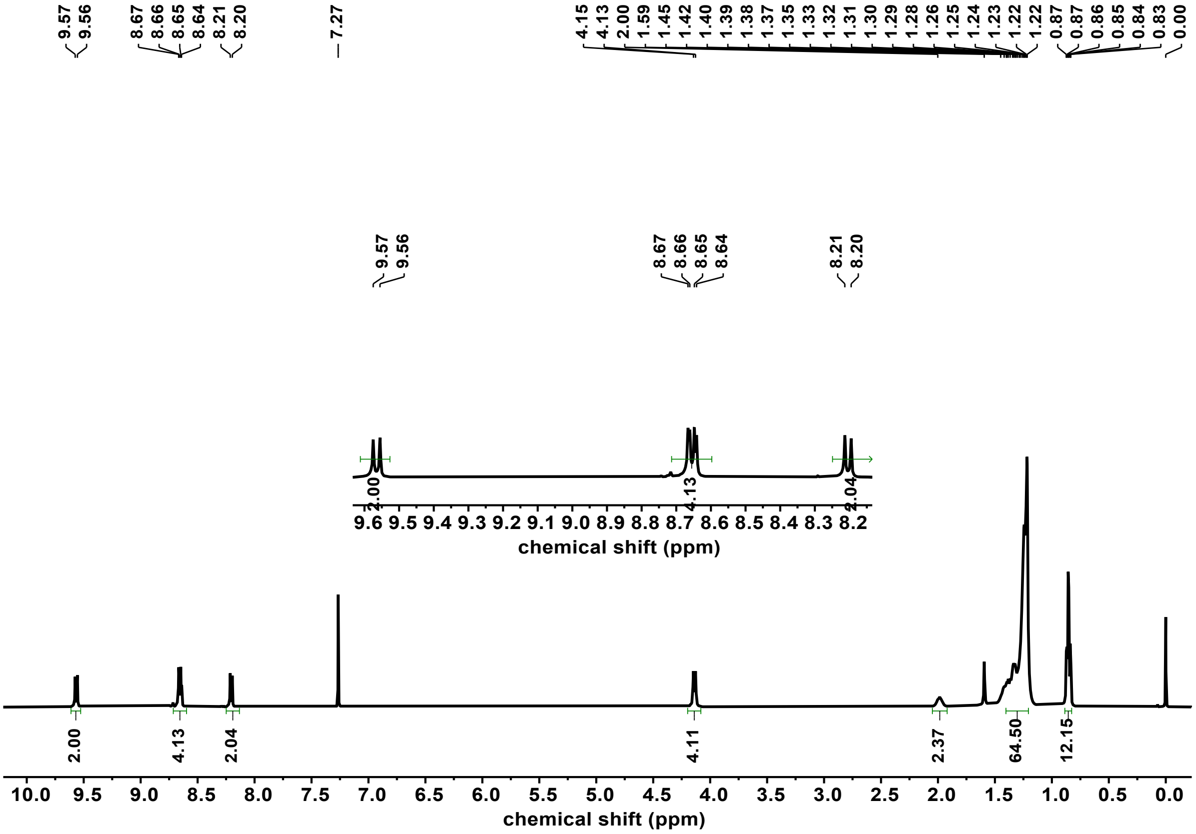


Figure S17. ^{1}H NMR spectrum of compound BAI-1 ($CDCl_3$, 40 °C).

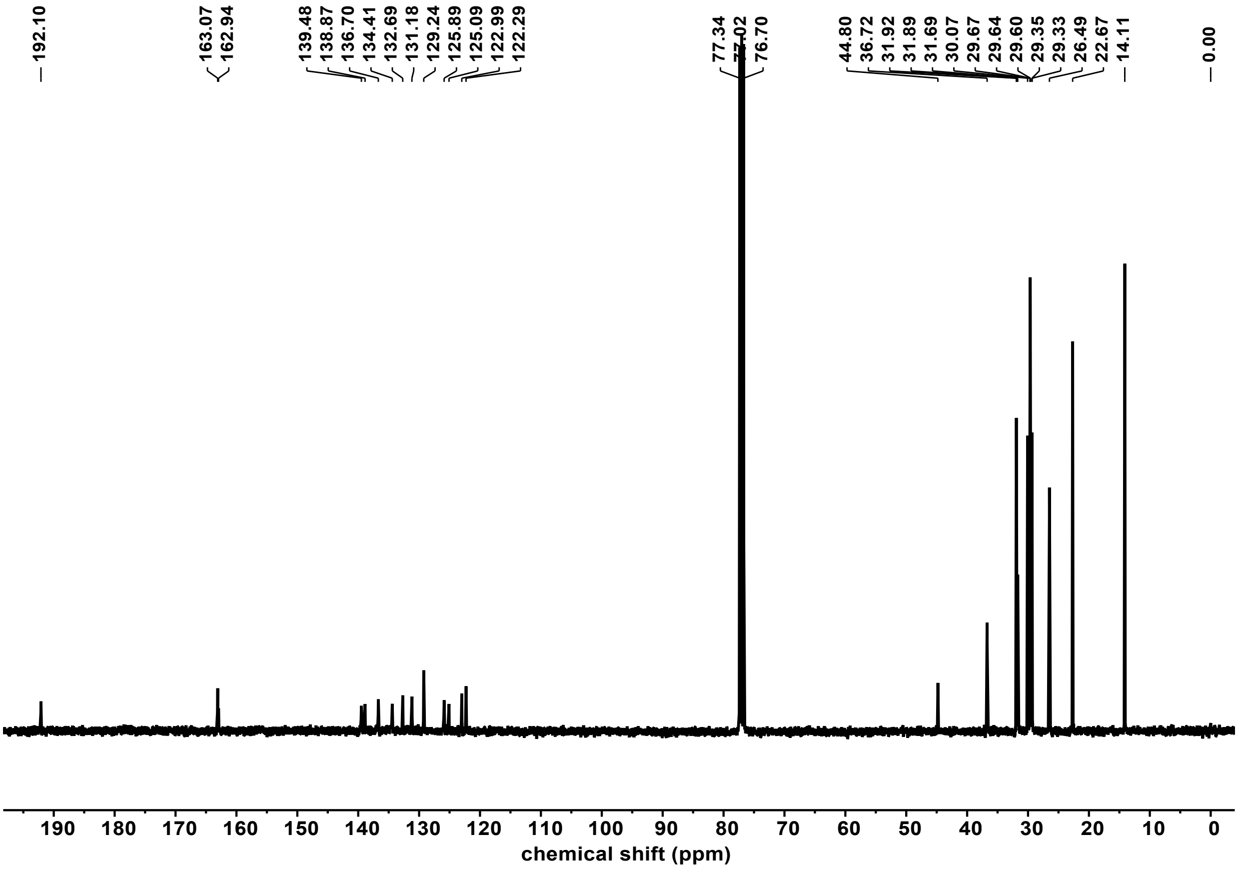


Figure S18. ^{13}C NMR spectrum of compound BAI-1 ($CDCl_3$, 25 °C).

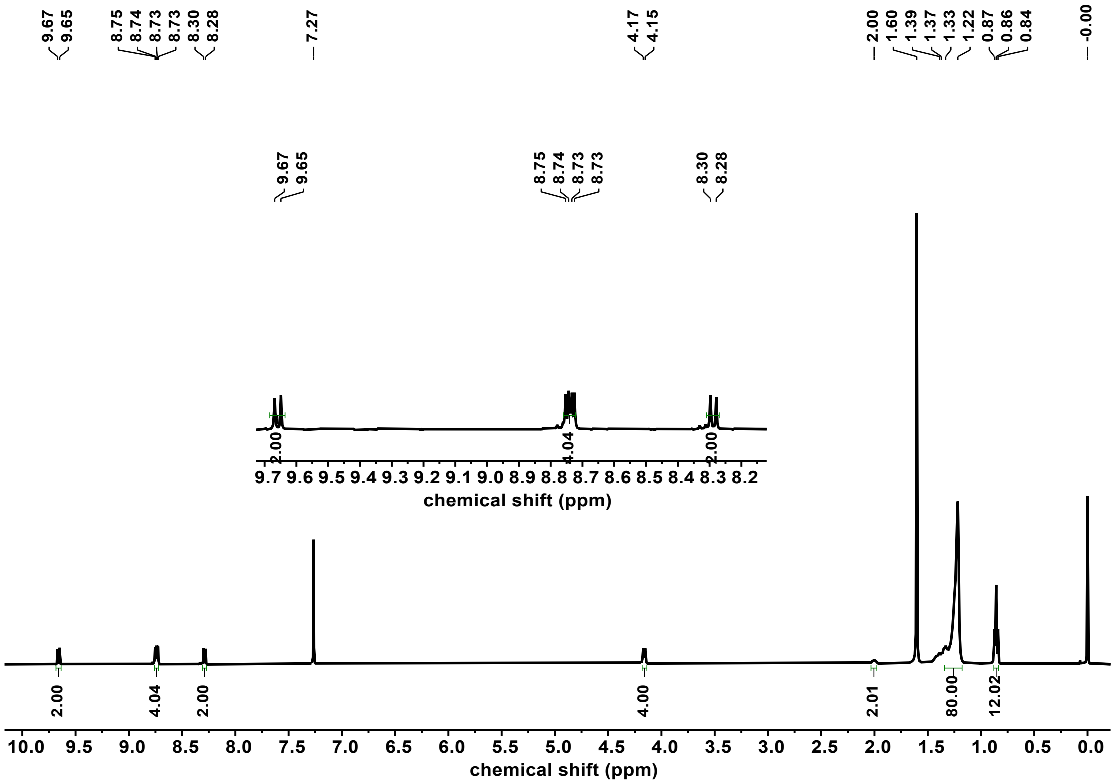


Figure S19. ^{1}H NMR spectrum of BAI-2 ($CDCl_3$, 40 °C).

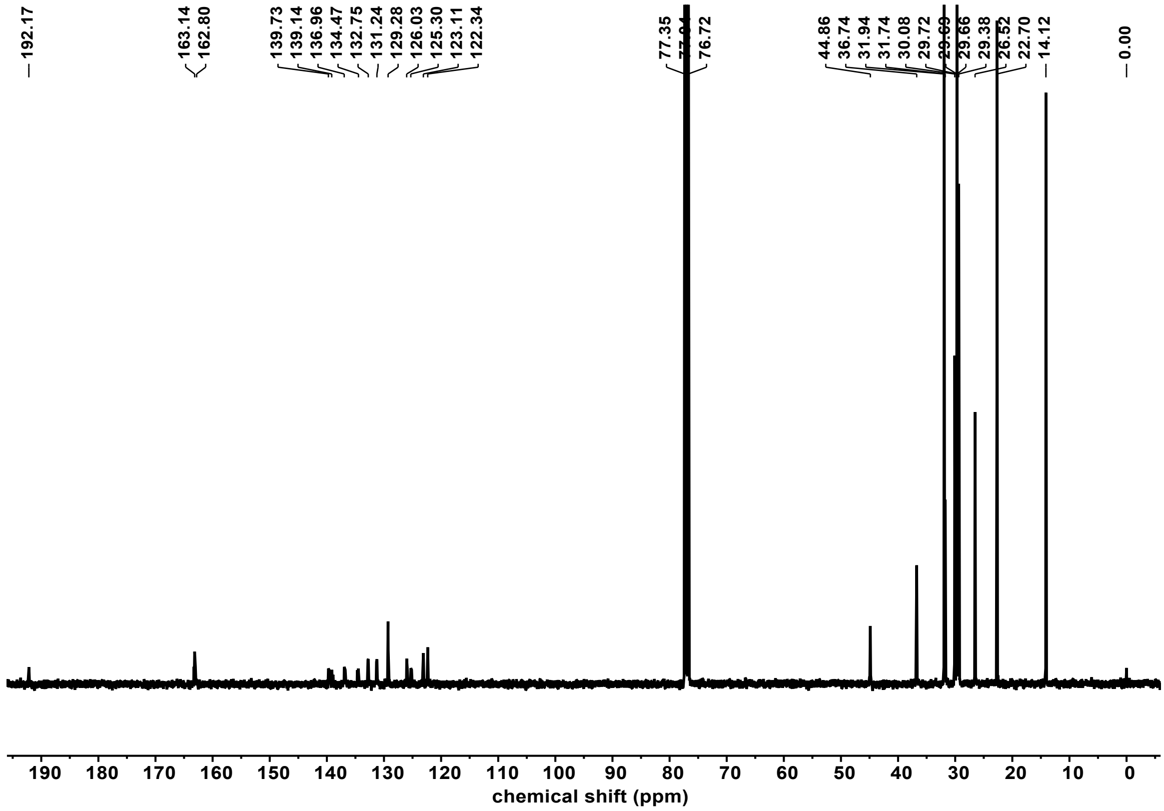


Figure S20. ^{13}C NMR spectrum of BAI-2 ($CDCl_3$, 25 °C).

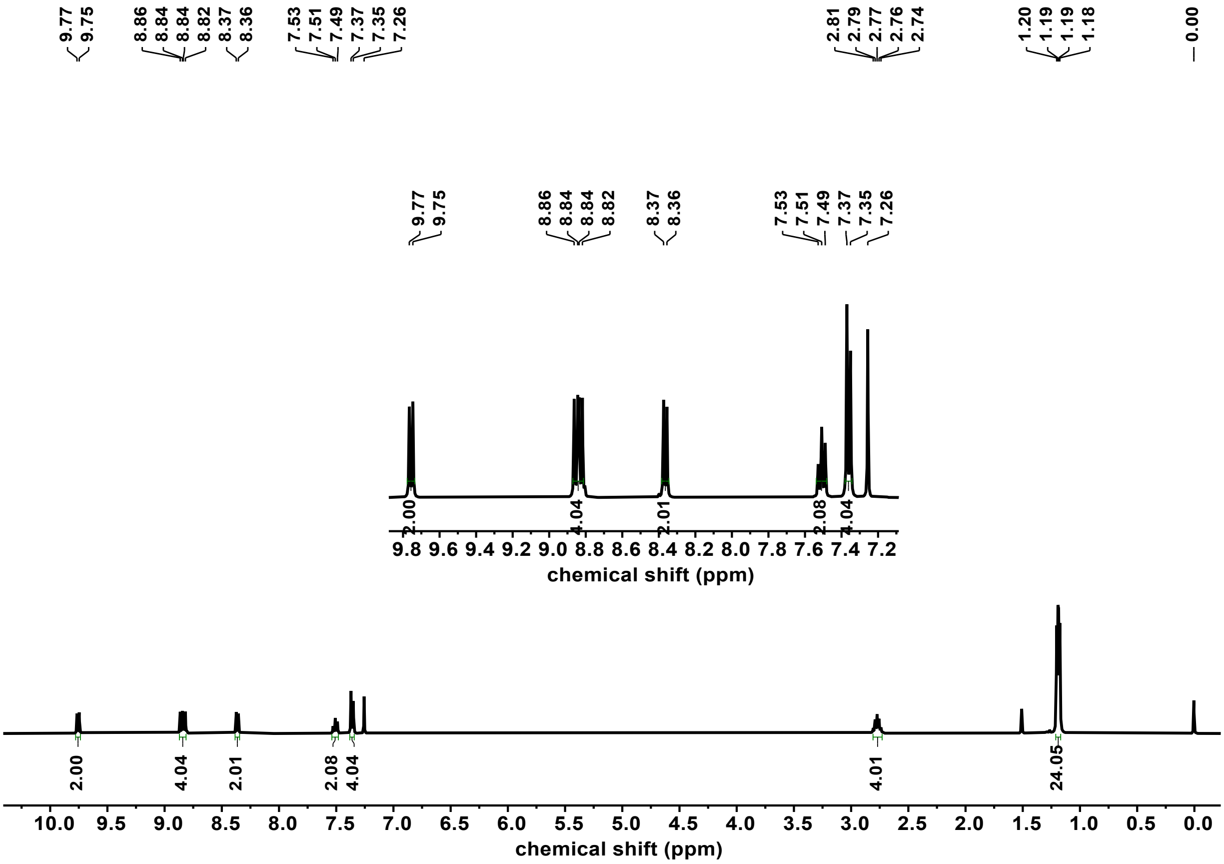


Figure S21. ^{1}H NMR spectrum of BAI-3 (CDCl$_3$, 40 °C).

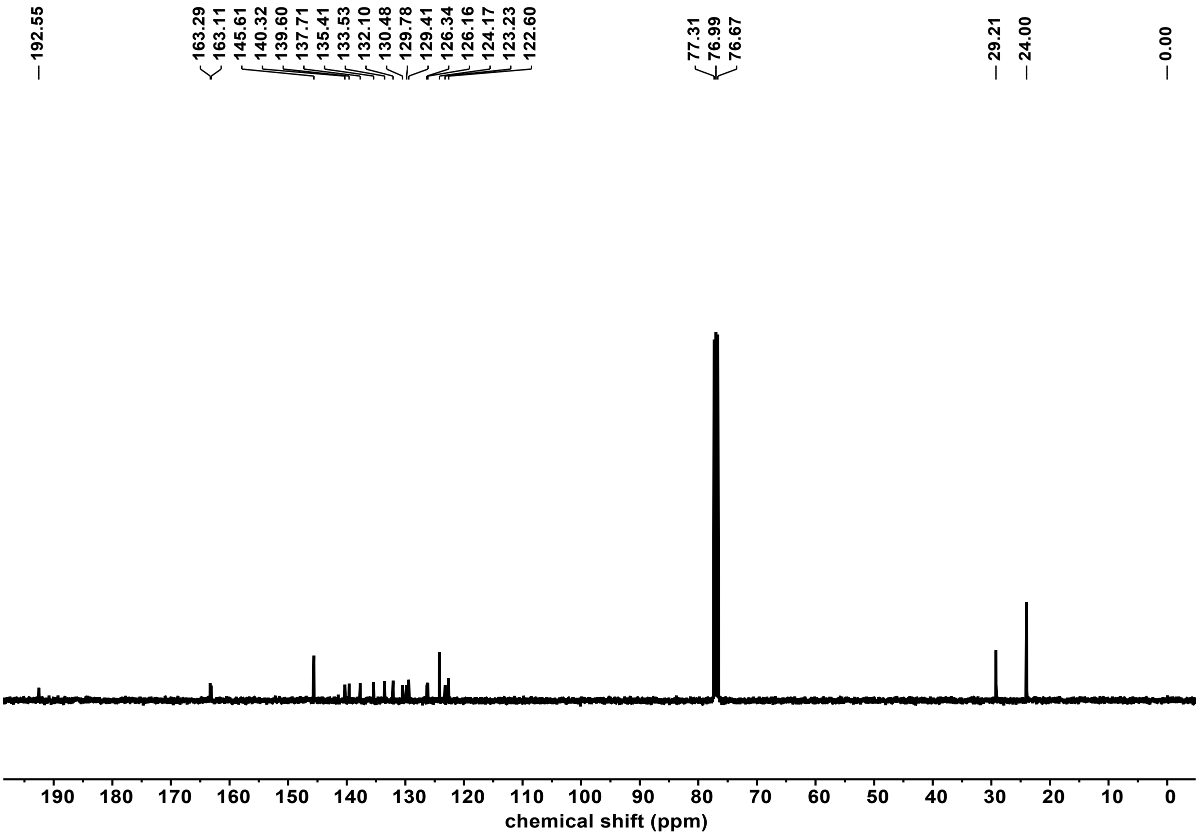


Figure S22. ^{13}C NMR spectrum of BAI-3 (CDCl$_3$, 25 °C).

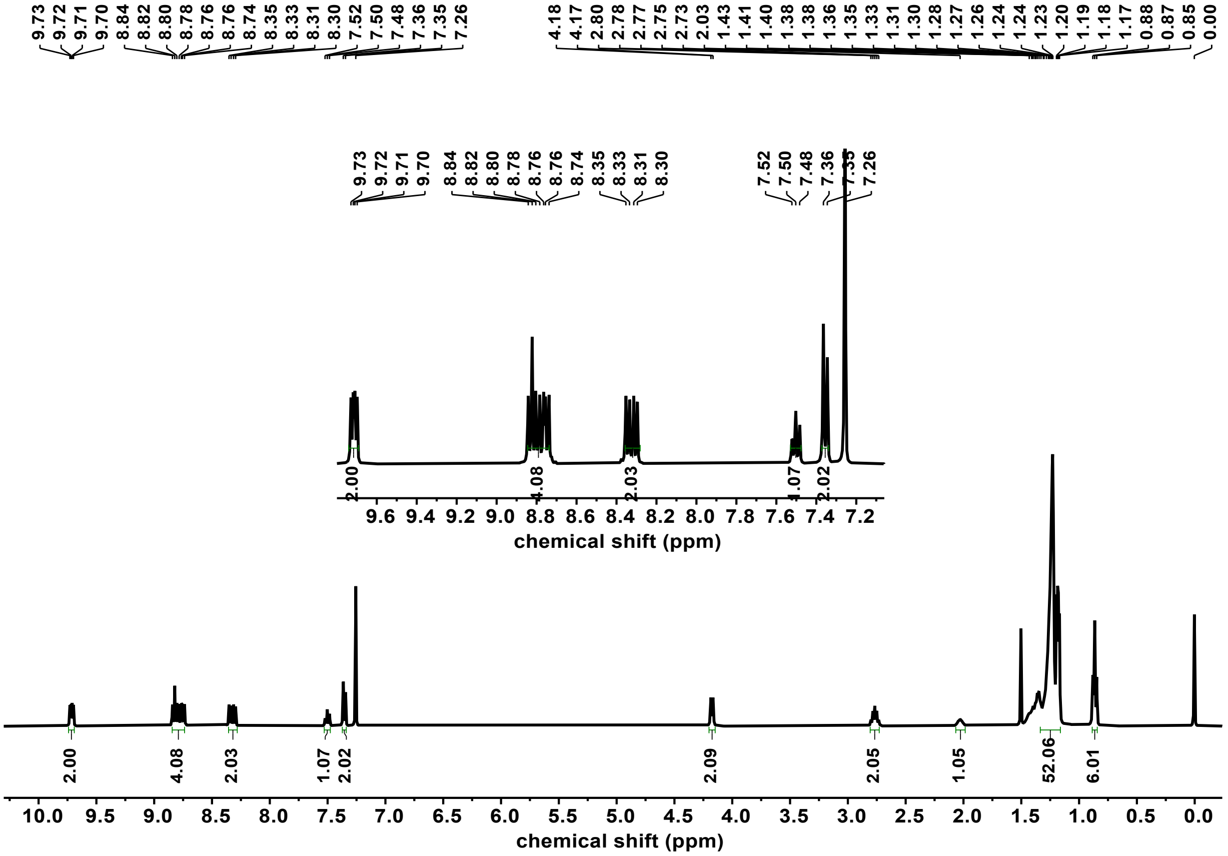


Figure S23. ^{1}H NMR spectrum of BAI-4 ($CDCl_3$, 40 °C).

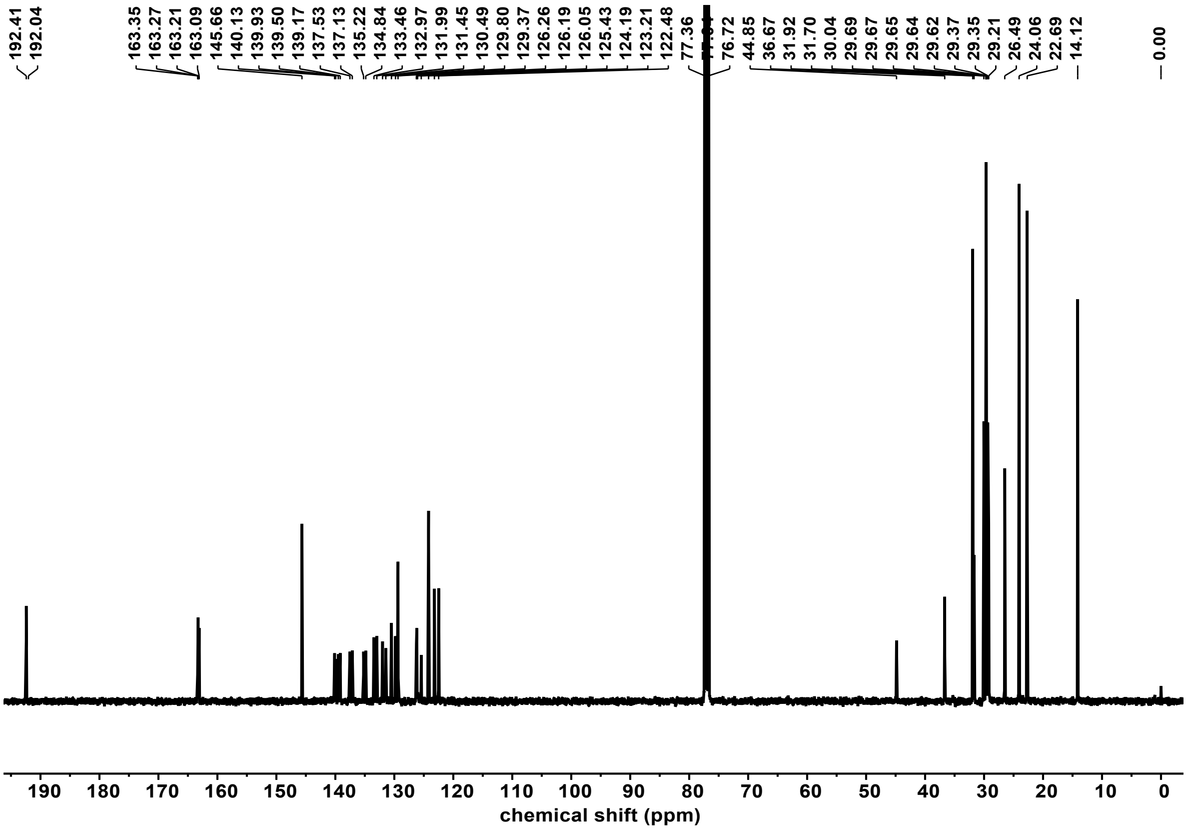


Figure S24. ^{13}C NMR spectrum of BAI-4 ($CDCl_3$, 25 °C).

11. Notes and References.

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